

Condensed Matter Theory

Matthew Gebert

May 8, 2020

A review of basic principles and exercises

Contents

0.1	Introduction to Quantum Transport - Datta & Purdue university, EdX	4
1	The Drude Theory of Metals	5
1.1	Summaries from Ashcroft / Mermin	5
1.1.1	Basic assumptions of the Drude model	5
1.1.2	DC electrical conductivity	6
1.1.2.1	In the presence of a magnetic field	7
1.1.2.2	In the presence of a time-varying electric field	7
1.1.3	Thermal Conductivity	7
1.1.3.1	Thermoelectric effect	8
1.2	Problems from Ashcroft / Mermin	9
1.2.1	Poisson Distribution	9
1.2.1.a)	Probability of no collision	9
1.2.1.b)	Probability of collision in small interval	9
1.2.1.c)	Mean time to next collision / previous collision using a)	9
1.2.1.d)	Mean time between collisions using b)	10
1.2.1.e)	Drude's mistakes	10
1.2.2	Joule Heating	11
1.2.2.a)	Average energy loss	11
1.2.2.b)	Average energy loss from Q1	11
1.2.3	Thomson Effect	12
1.2.4	Helicon Waves	12
1.2.4.a)	Circular polarisation	13
1.2.4.b)	Maxwell's equations soln	14
1.2.4.c)	Sketch of ϵ	16
1.2.4.d)	Estimation of Helicon frequency	16
1.2.5	Surface Plasmons	17
1.2.5.a)	Relate q , K and K'	17
1.2.5.b)	Plot	19
1.2.5.c)	The surface plasmon	19
2	The Sommerfeld Theory of Metals	21
2.1	21
2.1.1	Stat mech of thermal properties	22
2.1.2	Conduction Theory	23
2.1.3	Applications of Fermi-Dirac distribution	23
3	Quantum Transport	24
3.1	Introduction	24
3.1.1	Energy of an atom	24
3.1.2	Wave equation	25
3.1.2.1	Particle in a box	25
3.1.2.2	Crystals	26

Introduction

0.1 Introduction to Quantum Transport - Datta & Purdue university, EdX

- Diffusive - Drude Model

$$R = \frac{\rho}{A} L, \rho = \frac{m}{nq^2\tau} \quad (1)$$

- Ballistic (independent of length). Can you describe long devices? Yes you can, with an extra factor of the mean free path compared to the length.

$$R = \frac{h}{q^2} \frac{1}{M} \left(1 + \frac{L}{\lambda} \right) \quad (2)$$

- Atoms, quantum.

Chapter 1

The Drude Theory of Metals

1.1 Summaries from Ashcroft / Mermin

Understanding the metallic state leads to the understanding of insulators and other materials. Some models are very wrong in certain aspects, but are very useful for learning the progress of solid state physics over the last 100 plus years. Around 1900, Drude put forward a theory of metallic conduction. This had serious successes, and provides rough estimates for properties that are actually very complex. It goes without saying the failures are what drove and changed investigation of the theory of materials with the introduction of quantum theories into the mid 1900's.

1.1.1 Basic assumptions of the Drude model

The electron was only discovered in 1897, including the conduction of metals. He did this by applying the kinetic theory of gasses to that of electrons in a metal. The idea was that metallic elements brought together release delocalized electrons, while cations stay immobile.

Interestingly, the role of valence electrons form the *conduction electrons* rather than the general material valence band electrons (insulating). This naming is a bit odd.

Density For electrons with mass m , the number density is:

$$n = N_A \frac{Z \rho_m}{A} \quad (1.1)$$

where N_A is Avagadro's number, ρ_m is the mass density in grams/cm³, Z is the number of contributed valence electrons, and A is the atomic mass.

A radius can also be calculated per conduction electron, assuming a spherical volume.

$$\frac{V}{N} = \frac{1}{n} = \frac{4\pi r_s^3}{3} \quad (1.2)$$

Comparing these values for materials against the Bohr radius a_0 , we find that most metals (with some exceptions) fall between $r_s/a_0 = (2,3)$. Densities in gasses are typically 1000x greater. The Z values are arbitrarily selected through this model.

It turns out that electron-electron scattering doesn't contribute significantly to the total scattering amplitude, making the Drude model a good approximation in many places. This is fortunate because just assuming there is some scattering (regardless of the origin) can still provide an insight into metallic conduction.

Assumptions include

1. Forces only really in play during collision. No consideration of electrostatic forces. Neglecting electron-electron interaction is called *independent electron approximation*. Neglecting electron-ion interactions is called *free electron approximation*.
2. Collisions are abrupt. Drude attributed light negative charged electrons scattering off positive ions that are much heavier and

immobile. There was some scattering mechanism, and in this initial model it was the ion-electron kinematic collisions.

3. A collision occurs with probability per unit time $1/\tau$. Here τ is the relaxation time (also known as the mean free time or the collision time). This parameter is fundamental in metallic conduction. This time τ is taken to be independent of an electrons position or velocity, which should obviously be wrong but still turns out to make good predictions for many applications.
4. Thermal equilibrium comes about through collisions only. The particle scattering from a collision experiences a random direction and a speed appropriate to the temperature of the locality of the material. Hotter regions result in faster electrons.

1.1.2 DC electrical conductivity

Ohms law gives $V = IR$. Making this dimensionless, from resistance to resistivity, we have

$$\mathbf{V} = R\mathbf{I} \quad (1.3)$$

$$\rightarrow \mathbf{E} = \rho \mathbf{j} \quad (1.4)$$

If a density of n electrons per unit volume move with velocity \mathbf{v} , then the current density will be

$$\mathbf{j} = -ne\mathbf{v} \quad (1.5)$$

We can derive the average current and velocity of electrons after some characteristic time τ . Consider an electron at zero velocity. After some time τ , it has accelerated in the electric field to be moving at:

$$v_{final} = 0 + \int a_E dt \quad (1.6)$$

$$= -\frac{e\mathbf{E}}{m_e}\tau \quad (1.7)$$

and consequently the current density will be

$$\mathbf{j} = \left(\frac{ne^2\tau}{m}\right) \mathbf{E} \quad (1.8)$$

This allows us to write the conductivity as per Ohms law:

$$\mathbf{j} = \sigma \mathbf{E}, \sigma = \frac{ne^2\tau}{m} \quad (1.9)$$

Working backwards, experimentalists can use resistivity measurements to estimate the relaxation time. This can be written in terms of the value of r_s and a_0 and micro-ohm centimetres.

$$\tau = \frac{m}{\rho n e^2} = \left(\frac{0.22}{\rho_\mu}\right) \left(\frac{r_s}{a_0}\right)^3 \times 10^{-14} sec \quad (1.10)$$

In Drude's era using the equipartition theorem of statistical mechanics to assume the energy of a particle was very normal, and so the velocity was inferred by $\frac{1}{2}mv_0^2 = \frac{3}{2}k_B T$. This allowed the construction of a "mean free path", the average distance travelled before scattering, calculated as

$$\ell = v_0 \tau \quad (1.11)$$

Values for the mean free path were observed to be between 1 - 10 Å, which is very comparable to atomic spacing and a realistic view of his model. However this doesn't apply for all temperatures. There are issues at room temperature, where v_0 is a magnitude of order off, at lowest temperatures v_0 is off. We can work with mean free paths on the order of centimetres (compared to angstroms) strongly suggesting that it's not just a matter of "bumping off ions".

Without a good theory of collision time τ , it becomes important to find quantities that are independent of this parameter. The following two cases are of interest for the conductivity; a spatially uniform magnetic field, and a spatially uniform time varying electric field.

Consider the current density (Eq. 1.5) in terms of momentum $\mathbf{v} = \mathbf{p}/m$.

$$\mathbf{j} = -\frac{nep(t)}{m} \quad (1.12)$$

With some external force (electric/magnetic fields) $\mathbf{f}(t)$, then some infinitesimal time later, and given the probability that the electron hasn't collided, we have the following change in momentum:

$$\mathbf{p}(t+dt) = \left(1 - \frac{dt}{\tau}\right) [\mathbf{p}(t) + \mathbf{f}(t) + O(dt)^2] \quad (1.13)$$

$$= \mathbf{p}(t) - \frac{dt}{\tau} \mathbf{p}(t) + \mathbf{f}(t) + O(dt)^2 \quad (1.14)$$

This is just keeping to first order. Re-arranging and taking the limit $dt \rightarrow 0$ we have:

$$\frac{\mathbf{p}(t+dt) - \mathbf{p}(t)}{dt} = \frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t) \quad (1.15)$$

1.1.2.1 In the presence of a magnetic field

We have introduced field \mathbf{H} , which gives a Lorentz force to the electron

$$\mathbf{F}_{cgs} = -\frac{e}{c} \mathbf{v} \times \mathbf{H} \quad (1.16)$$

Two important quantities arise, the magnetoresistance and the Hall resistance:

$$\rho(H) = \frac{E_x}{j_x}, R_H = \frac{E_y}{j_x H} \quad (1.17)$$

Note that early experiments by Hall showed that some metals actually have a positive Hall coefficient H , which implies a different charge carrier to the negative electron.

- Drude Predicts temperature independent and density independent Hall resistance.
- Quantum theory of solids is needed instead.
- The cyclotron frequency is also an important quantity in the Drude theory for a magnetic field.

1.1.2.2 In the presence of a time-varying electric field

- Substitute in an electric field $\text{Re}(\mathbf{E}(\omega)e^{-i\omega t})$
- Solve for ohms law, find $\sigma(\omega)$
- Reduces to DC Drude result.
- If with magnetic field of same magnitude, H field can be ignored due to weakness.
- Varying E fields in space? These can't be ignored as easily. But can get away with by knowing that majority of collisions occur near the original point of the field considered. If the field varies slowly at this length scale, then the approximation is correct. (Field $\lambda > \ell$)
- Solving Maxwell's equations gives exponential decaying solutions below a critical frequency, and propagation above.
- If propagating, then transparency can be observed, and this has been seen and predicted in alkali metals.

- Realistically, the dielectric function is much more complex, and terms do compete substantially with the Drude term.
- Plasma oscillations or plasmons are charge density oscillations that can occur in a metal, as above, and are established above the critical frequency.

1.1.3 Thermal Conductivity

- The Wiedemann and Franz law (1853) states κ/σ which is the ratio of thermal to electrical conductivity is directly proportionate to the temperature.
- Drude explained this using the idea that thermal current is much more significant in electrons than in ions.
- Scenario - Bar with hot end, loses heat to cold end, but also give hot end amount of heat it loses.
- $j^q = -\kappa \nabla T = -\kappa \frac{dT}{dx}$
- Hotter electrons will have higher energies leading to a net flow of thermal energy.
- Each electron will carry thermal energy $\mathcal{E}(T[x - vt])$ based on how far it travels before colliding.
- At some point, half come from hot, half from low. Evaluating the thermal current gives

$$\mathbf{j}^q = \frac{1}{3} v^2 \tau c_v (-\nabla T) \quad (1.18)$$

- Ashcroft and Mermin emphasise the roughness of this argument, given the vagueness about thermal energy, thermal averages, speed of electrons, etc.
- Drude used the ideal gas laws to go further and eventually work out the ratio of $\frac{\kappa}{\sigma}$. He achieved a result a factor half from the experimental observations, which is pretty remarkable (originally left out the factor of half erroneously).
- Two issues with this include 1) room temperature electronic contribution to specific

heat is 100x smaller than this classical prediction. 2) Mean square electronic speed is about 100x larger.

- Even the assumption of thermally dependent particle energies is wrong, but its correction only alters the result by factor of order unity making this a good assumption.

1.1.3.1 Thermoelectric effect

- Consider a circuit, with a temperature gradient. Because it's a open circuit, no charge current can flow.
- However, because the material bar has a temperature gradient, electrons on one side have higher velocity and have net drift, ie net current.

- Consequently an electric field should direct opposite to the temperature gradient.

- Seebeck effect:

$$\mathbf{E} = Q \nabla T \quad (1.19)$$

Q is thermopower.

- We can find the thermopower by evaluating the velocity due to the temperature against the velocity due to an electric field. We find that the thermopowers are a factor 100 smaller uncompensated.
- Some metals have opposite sign to what Drude predicts though, and this can be calculated but there is still a lack of quantitative thermoelectric fields.

1.2 Problems from Ashcroft / Mermin

1.2.1 Poisson Distribution

In the Drude model, the probability of an electron suffering a collision in an infinitesimal time dt is dt/τ .

1.2.1.a) Probability of no collision

Show that an electron picked at random at a given moment had no collision during the preceding t seconds with probability $e^{-t/\tau}$. Show that it will have no collision during the next t seconds with the same probability.

We need to derive that the process is actually a Poisson distribution. Consequently, we know that in a very small time the probability of a collision is dt/τ . The probability of avoiding a collision is then:

$$\rho_{\text{avoid}} = 1 - \frac{dt}{\tau} \quad (1.20)$$

If we have some time t , we can break it up into N parts, and let N approach infinity to satisfy the infinitesimal quantity.

By multiplying the probability of avoiding collision with N segments of infinitesimal time together, we get:

$$\rho_{\text{avoid}}(t) = \left(1 - \frac{\Delta t}{\tau}\right)^N = \left(1 - \frac{t}{N\tau}\right)^N \quad (1.22)$$

Here we can use a limit theorem,

$$\lim_{x \rightarrow \infty} \left(1 + \frac{a}{x}\right)^x = e^a \quad (1.23)$$

and so we have

$$\frac{t}{N} = \Delta t, \lim_{N \rightarrow \infty} (\Delta t) = dt \quad (1.21)$$

$$\lim_{N \rightarrow \infty} \rho_{\text{avoid}}(t) = e^{-t/\tau} \quad (1.24)$$

1.2.1.b) Probability of collision in small interval

Show that the probability that the time interval between two successive collisions of an electron falling in the range between t and $t+dt$ is $(dt/\tau)e^{-t/\tau}$.

We already have the probability of not colliding by time t . The probability of a collisions after infinitesimal time dt is given from the introduction dt/τ . Therefore the probability of colliding at some time small interval of time is given by:

$$\rho_{t \rightarrow t+dt} = \rho_{\text{avoid}}(t) \times \rho_{\text{collide}}(dt) \quad (1.25)$$

$$= e^{-t/\tau} \left(\frac{dt}{\tau}\right) \quad (1.26)$$

Note it may be tempting to calculate the probability of colliding within an interval as

$$1 - \frac{1}{\tau} \int_t^{t+dt} e^{-t'/\tau} dt' \quad (1.27)$$

but note that this includes multiple new collisions, not just a single collision.

1.2.1.c) Mean time to next collision / previous collision using a)

Show that as a consequence of (a) that at any moment the mean time back to the last collision (or up to the next collision) averaged over all electrons is τ .

The expectation value of a probability distribution function (PDF) for x is given by the inte-

gral:

$$\text{Exp}(x) = \int_0^{\infty} x \times \text{PDF}(x) dx \quad (1.28)$$

We have already found the PDF in part sec-

tion 1.2.1.a), but need to multiply a normalisation factor $\frac{1}{\tau}$. Using the integration by parts, $xe^{-ax}dx = -\frac{x}{a}e^{-ax} + \frac{1}{a}e^{-ax}dx$, we can evaluate the integral:

$$\langle t \rangle = \frac{1}{\tau} \int_0^\infty te^{-t/\tau} dt \quad (1.29)$$

1.2.1.d) Mean time between collisions using b)

Show as a consequence of (b) that the mean time between successive collisions of an electron is τ .

This question seems a little redundant and I'm not quite sure what the purpose of it is.

In section 1.2.1.b) we found the probability of no collisions then a collision is:

$$p_{t \rightarrow t+dt} = e^{-t/\tau} \left(\frac{dt}{\tau} \right) \quad (1.32)$$

$$= \frac{1}{\tau} \left[-(t\tau)^{-t/\tau} \right]_0^\infty + \frac{1}{\tau} \int_0^\infty \tau e^{-t/\tau} dt \quad (1.30)$$

$$= 0 + \left[-\tau e^{-t/\tau} \right]_0^\infty = \tau \quad (1.31)$$

Using this result, we can find the average time as:

$$\langle t \rangle = \int_0^\infty te^{-t/\tau} \left(\frac{1}{\tau} \right) dt \quad (1.33)$$

However this is the same integral as in section 1.2.1.c), so the result is the same.

1.2.1.e) Drude's mistakes

Part (c) implies that any moment the time T between the last and next collision averaged over all electrons is 2τ . Explain why this is not inconsistent with the result in (d) (A thorough explanation should include a derivation of the probability distribution for T). A failure to appreciate this subtlety led Drude to a conductivity only half of (Eq1.6, Ashcroft & Mermin). He did not make the same mistake in the thermal conductivity, whence the factor of two in his calculation of the Lorenz number.

To deriving the probability distribution for T , we need to recognise it's the join distribution of two distributions, which implies convolving the

two links between the time to the previous and the time to the next, consequentially integrate over a intermediate time t_1 .

$$P(T) = \int_0^T e^{-(T-t_1)/\tau} \left(\frac{1}{\tau} \right) \times e^{-t_1/\tau} \left(\frac{dt_1}{\tau} \right) \quad (1.34)$$

$$= \int_0^T e^{-T/\tau} \left(\frac{1}{\tau^2} \right) dt_1 \quad (1.35)$$

$$= \frac{T e^{-T/\tau}}{\tau^2} \quad (1.36)$$

The expectation of such a distribution is as follows:

$$\langle T \rangle = \int_0^\infty T P(T) dT \quad (1.37)$$

$$= \int_0^\infty T \frac{T e^{-T/\tau}}{\tau^2} dT \quad (1.38)$$

$$= \left[-\tau \frac{T^2}{\tau^2} e^{-T/\tau} \right]_0^\infty + 2 \int_0^\infty \frac{T e^{-T/\tau}}{\tau} dT \quad (1.39)$$

First bounded term disappears,

$$\begin{aligned} \text{substitute } T = -\tau \log(u), dT = -\tau \frac{1}{u} du \\ = 0 + 2 \int_1^0 \frac{T}{\tau} u \times \frac{-\tau}{u} du \end{aligned} \quad (1.40)$$

$$= 2 \int_0^1 T du = -2\tau \int_0^1 \log(u) du \quad (1.41)$$

$$= -2\tau [-u + u \log(u)]_0^1 = 2\tau \quad (1.42)$$

The result above is as expected.

The result is not inconsistent with (d) because the probability from *any* time to the next collisions is always the same. Therefore it is a result of choosing the initial condition of being from a collisions that has just occurred, or in between two

collisions, where no collision has occurred. Because Poisson like distributions don't keep track of past events, the expectation time till the next

collision is always same no matter the initial condition.

1.2.2 Joule Heating

Consider a metal at a uniform temperature in a static uniform electric field \mathbf{E} . An electron experiences collision, and then, after a time t , a second collision. In the Drude model, energy is not observed in collisions, for the mean speed of an electron emerging from a collision does not depend on the energy that the electron acquired from the field since the time of the preceding collision.

1.2.2.a) Average energy loss

Show that the average energy lost to the ions in the second of two collisions separated by a time t is $(e\mathbf{E}t)^2/2m$. (The average is over all directions in which the electron emerged from the first collision)

If the time between collisions is t , then the acceleration on the object is

$$= \frac{-e\mathbf{E}t}{m_e} \quad (1.45)$$

$$\mathbf{a}_E = \frac{-e\mathbf{E}}{m_e} \quad (1.43)$$

Calculating the kinetic energy:

Calculating gained velocity:

$$\delta E_k = \frac{1}{2}m_e \left(\frac{-e\mathbf{E}t}{m_e} \right)^2 \quad (1.46)$$

$$\Delta v = \int_0^t \mathbf{a}_E dt \quad (1.44)$$

$$= \frac{(e\mathbf{E}t)^2}{2m_e} \quad (1.47)$$

1.2.2.b) Average energy loss from Q1

Show using the result of section 1.2.1.b) that the average energy loss to the ions per electron per collision is $(e\mathbf{E}\tau)^2/m$, and hence that the average loss per cubic centimetre per second is $(ne^2\tau/m)\mathbf{E}^2 = \sigma\mathbf{E}^2$. Deduce that the power loss in a wire of length L and cross section A is I^2R , where I is the current flowing, and R is the resistance.

We know from Drude theory that the DC conductivity of a metal under the influence of an electric field can be calculated from the net acceleration each particle experiences before a collision. Using the averaged collision time τ this gives an average velocity and in turn a net conductivity:

$$j = -nev \quad (1.48)$$

$$v_{avg} = \frac{v_f - v_i}{2} = \left(\frac{-eE}{m_e}\tau - 0 \right) / 2 \quad (1.49)$$

$$\Rightarrow j = -\frac{ne^2\tau}{2m_e}E \quad (1.50)$$

$$\sigma = \frac{ne^2\tau}{2m} \quad (1.51)$$

From question 1, we have the probability of two successive collisions falling between t and $t+dt$ is $(dt/\tau)e^{-t/\tau}$.

using Q1? Unclear.

To calculate the loss per cubic centimetre, recognise there are n conduction electrons per cubic centimetre, and these on average collide every τ seconds. Then the energy loss is per cubic centimetre per second is:

$$\frac{dE}{dt} = n \times \Delta E / \tau = \frac{ne^2\tau}{m}E^2 = \sigma E^2 \quad (1.52)$$

Following this, we know that in a wire with cross section A and length L , that there will be a power loss of

$$P = L \times A \times \frac{dE}{dt} \quad (1.53)$$

$$= AL \times \frac{ne^2\tau}{m}E^2 = AL \times \sigma E^2 \quad (1.54)$$

Figure out how to generate same result but

Note that adding in dimensional factors to ohms

law gives:

$$V = RI \quad (1.55)$$

$$\left(\frac{V}{L}\right) = \left(\frac{A}{L}R\right) \left(\frac{I}{A}\right) \quad (1.56)$$

$$E = \frac{1}{\sigma}J \quad (1.57)$$

Recognising the same terms in eq. (1.54), we then

have:

$$P = AL \times \sigma E^2 \quad (1.58)$$

$$= \frac{A^2 L}{A} \frac{\sigma^2}{\sigma} E^2 \quad (1.59)$$

$$= (Aj)^2 \left(\frac{L}{A\sigma}\right) = I^2 R \quad (1.60)$$

1.2.3 Thomson Effect

Suppose that in addition to the applied electric field in Problem 2 there is also a uniform temperature gradient ∇T in the metal. Since an electron emerges from a collision at an energy determined by the local temperature, the energy lost in collisions will depend on how far down the temperature gradient the electron travels between collisions, as well as on how much energy it has gained from the electric field. Consequently the power lost will contain a term proportional to $\mathbf{E} \cdot \nabla T$ (which is easily isolated from the other terms since it is the only term in the second-order energy loss that changes sign when the sign of \mathbf{E} is reversed). Show that this contribution in the Drude model by a term of order $(ne\tau/m)(d\mathcal{E}/dT)(\mathbf{E} \cdot \nabla T)$, where \mathcal{E} is the mean thermal energy per electron. (Calculate the energy lost by a typical electron collision at \mathbf{r} , which made its last collision at $\mathbf{r} - \mathbf{d}$). Assuming a fixed, energy-independent relaxation time τ , \mathbf{d} can be found to be linear in order in the field and temperature gradient by simple kinematic arguments which is enough to give the energy loss to second order.)

To show the additional term, consider the energy lost over some temperature gradient via the Drude model. In the original Drude model, we had particles colliding at some uniform temperature, scattering with a new velocity/direction proportional to the temperature. This temperature now has a gradient.

Say the electron starts at some position with temperature / energy \mathcal{E}_i and moves through temperature to a new temperature corresponding to energy \mathcal{E}_f . On average without an electric field, velocity is random and so energy is gained or lost in equal amounts as the particle "collides" according to the Drude model either side of the gradient.

However, in the presence of an electric field, the average velocity is non-zero, and so there is a net movement of thermal energy, which depends on the dot product of the electric field and the uniform temperature gradient.

Repeating the calculation from Q2 for the average velocity gained in collision time τ we have

$$\mathbf{v} = \int_0^\tau \frac{-e\mathbf{E}}{m_e} dt \quad (1.61)$$

$$= -\frac{e\mathbf{E}\tau}{m_e} \quad (1.62)$$

We do not need to find the distance travelled before a second collision, because it's rather the rate of motion across temperature, across a change in the thermal energy of electrons, that implies a loss of energy per unit time.

Therefore considering the power loss of a single electron, it's velocity determines how far it moves across a temperature gradient $\nabla_d T$ through space, which in turn determines how much the thermal energy \mathcal{E} of the particle will change.

$$\nabla P = \mathbf{v} \cdot \nabla T \times \frac{d\mathcal{E}}{dT} \quad (1.63)$$

$$= \frac{-e\mathbf{E}\tau}{m_e} \cdot \nabla T \times \frac{d\mathcal{E}}{dT} \quad (1.64)$$

$$= \frac{-e\tau}{m_e} \left(\frac{d\mathcal{E}}{dT}\right) (\mathbf{E} \cdot \nabla T) \quad (1.65)$$

It is simple to add in the factor n , which is the number of electrons.

1.2.4 Helicon Waves

Suppose that a metal is placed in a uniform magnetic field \mathbf{H} along the z -axis. Let an AC electric field $\mathbf{E}e^{-i\omega t}$ be applied perpendicular to \mathbf{H} .

1.2.4.a) Circular polarisation

If the electric field is circularly polarized ($E_y = \pm iE_x$) show that Eq. (1.28) must be generalised to

$$j_x = \left(\frac{\sigma_0}{1 - i(\omega \mp \omega_c)\tau} \right) E_x \quad (1.66)$$

Attempt at dynamic solution If the momentum of the electrons is influenced by an AC electric field and a constant magnetic field, we can consider the new equation of motion for the electrons.

$$\frac{d\mathbf{p}}{dt} = -e\mathbf{E} - \frac{e\mathbf{p}}{m_e c} \times \mathbf{H} - \frac{\mathbf{p}}{\tau} \quad (1.67)$$

Note that the last term comes from the infinitesimal probability of considering electrons that don't crash (ie, $1 - \frac{dt}{\tau}$), and neglecting second order terms that contribute to the Lorentz force components. Here our electric field has the form

$$\mathbf{E}(t) = \begin{bmatrix} E_x \\ E_y \end{bmatrix} e^{-i\omega t} \quad (1.68)$$

$$= \begin{bmatrix} E_x \\ \pm iE_x \end{bmatrix} e^{-i\omega t} \quad (1.69)$$

Noting $\hat{y} \times \hat{z} = \hat{x}$ and $\hat{x} \times \hat{z} = -\hat{y}$ Calculating the components, where $\omega_c = \frac{eH_z}{m_e c}$, we have

$$\frac{dp_x}{dt} = -eE_x e^{-i\omega t} - \omega_c p_y - \frac{p_x}{\tau} \quad (1.70)$$

$$\frac{dp_y}{dt} = -eE_y e^{-i\omega t} + \omega_c p_x - \frac{p_y}{\tau} \quad (1.71)$$

The dynamical solution for these simultaneous equations, solved through Mathematica is

$$p_x(t) = \frac{e\tau E_y}{\tau\omega_c - 1} e^{-it\omega} \quad (1.72)$$

Solving the equations by substituting p_y ,

$$\left(-i\omega + \frac{1}{\tau} \right) p_x(\omega) = -eE_x(\omega) - \omega_c \frac{-eE_y(\omega) + \omega_c p_x(\omega)}{(-i\omega + \frac{1}{\tau})} \quad (1.80)$$

$$\left(-i\omega + \frac{1}{\tau} + \frac{\omega_c^2}{(-i\omega + \frac{1}{\tau})} \right) p_x(\omega) = -eE_x(\omega) - \omega_c \frac{-eE_y(\omega)}{(-i\omega + \frac{1}{\tau})} \quad (1.81)$$

$$\left(\left(-i\omega + \frac{1}{\tau} \right) \left(-i\omega + \frac{1}{\tau} \right) + \omega_c^2 \right) p_x(\omega) = \left(-i\omega + \frac{1}{\tau} \right) \left(-eE_x(\omega) - \omega_c \frac{-eE_y(\omega)}{(-i\omega + \frac{1}{\tau})} \right) \quad (1.82)$$

$$\left(-\omega^2 - 2i\frac{\omega}{\tau} + \frac{1}{\tau^2} + \omega_c^2 \right) p_x(\omega) = -e \left(-i\omega + \frac{1}{\tau} \right) E_x(\omega) + e\omega_c E_y(\omega) \quad (1.83)$$

$$\left(-\omega^2 - 2i\frac{\omega}{\tau} + \frac{1}{\tau^2} + \omega_c^2 \right) p_x(\omega) = -e \left(-i\omega + \frac{1}{\tau} \mp i\omega_c \right) E_x(\omega) \quad (1.84)$$

$$p_y(t) = \frac{(eE_x - eE_y - e\tau\omega_c E_x)}{\omega_c(\tau\omega_c - 1)} e^{-it\omega} \quad (1.73)$$

Consequently, we can now multiply both sides by the factor ne/m to convert the momentum of an electron to the current density. However, this doesn't yield the target equation, and so we instead need to look towards the steady state solution as demonstrated on page 16 of Ashcroft & Mermin.

Attempt at steady state solution Treat the electric field and the momentum as a time and frequency dependent component.

$$E(t) = E(\omega) e^{-i\omega t} \quad (1.74)$$

$$p(t) = p(\omega) e^{-i\omega t} \quad (1.75)$$

Then substituting into the same equation of motion, we have:

$$-i\omega p_x(\omega) = -eE_x(\omega) - \omega_c p_y - \frac{p_x}{\tau} \quad (1.76)$$

$$-i\omega p_y(\omega) = -eE_y(\omega) + \omega_c p_x - \frac{p_y}{\tau} \quad (1.77)$$

Rearranging:

$$\left(-i\omega + \frac{1}{\tau} \right) p_x(\omega) = -eE_x(\omega) - \omega_c p_y(\omega) \quad (1.78)$$

$$\left(-i\omega + \frac{1}{\tau} \right) p_y(\omega) = -eE_y(\omega) + \omega_c p_x(\omega) \quad (1.79)$$

$$p_x(\omega) = \frac{-e(1 - i(\omega \mp \omega_c)\tau)}{\tau(-\omega^2 - 2i\frac{\omega}{\tau} + \frac{1}{\tau^2} + \omega_c^2)} E_x(\omega) \quad (1.85)$$

Note here that we can factor the denominator as such:

$$\left(\omega_c^2 - \omega^2 - 2i\frac{\omega}{\tau} + \frac{1}{\tau^2}\right) = \left(\frac{1}{\tau} - i\omega\right)^2 + \omega_c^2 \quad (1.86)$$

$$= \left(\frac{1}{\tau} - i\omega + i\omega_c\right) \left(\frac{1}{\tau} - i\omega - i\omega_c\right) \quad (1.87)$$

$$= \frac{1}{\tau^2} (1 - i(\omega + \omega_c)\tau) (1 - i(\omega - \omega_c)\tau) \quad (1.88)$$

$$= \frac{1}{\tau^2} (1 - i(\omega \pm \omega_c)\tau) (1 - i(\omega \mp \omega_c)\tau) \quad (1.89)$$

Cancelling the common factors provides the result:

$$p_x(\omega) = \frac{-e\tau}{(1 - i(\omega \pm \omega_c)\tau)} E_x(\omega) \quad (1.90)$$

Multiplying by the factor $\frac{ne}{m_e}$ to get the current density, we have

$$j_x(\omega) = \left(\frac{ne^2\tau}{m_e}\right) \frac{1}{1 - i(\omega \pm \omega_c)\tau} E_x(\omega) \quad (1.91)$$

$$= \frac{\sigma_0}{1 - i(\omega \pm \omega_c)\tau} E_x(\omega) \quad (1.92)$$

Note the \pm seems to be the wrong sign, but I can't find the sign error in this working.

1.2.4.b) Maxwell's equations soln

Show that, in conjunction with (1.61), Maxwell's equation (1.31) have a solution

$$E_x = E_0 e^{i(kz - \omega t)}, E_y = \pm i E_x, E_z = 0 \quad (1.93)$$

provided that $k^2 c^2 = \epsilon \omega^2$ where

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega} \left(\frac{1}{\omega \mp \omega_c + i/\tau} \right) \quad (1.94)$$

Maxwell's Equations Generally, in Gaussian units: can be written as

$$\nabla \cdot \mathbf{E} = 4\pi\rho \quad (1.95) \quad \nabla \cdot \mathbf{E} = 0 \quad (1.99)$$

$$\nabla \cdot \mathbf{H} = 0 \quad (1.96) \quad \nabla \cdot \mathbf{H} = 0 \quad (1.100)$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} \quad (1.97) \quad \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} \quad (1.101)$$

$$\nabla \times \mathbf{H} = \frac{1}{c} \left(4\pi \mathbf{J} + \frac{\partial \mathbf{E}}{\partial t} \right) \quad (1.98) \quad \nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{j} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} \quad (1.102)$$

Because we're looking at metals, there are no bound charges. Therefore Maxwells equation's Taking the curl of Faraday's law of induction, using the zero divergence property, and assuming

solutions that have $e^{-i\omega t}$ time dependence,

$$\nabla \times (\nabla \times \mathbf{E}) = \nabla \times \left(-\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} \right) \quad (1.103)$$

$$\nabla (\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} = -\frac{1}{c} \left(\nabla \times \frac{\partial \mathbf{H}}{\partial t} \right) \quad (1.104)$$

$$0 - \nabla^2 \mathbf{E} = \frac{i\omega}{c} (\nabla \times \mathbf{H}) \quad (1.105)$$

$$\nabla^2 \mathbf{E} = -\frac{i\omega}{c} \left(\frac{4\pi}{c} \mathbf{j} - \frac{i\omega}{c} \mathbf{E} \right) \quad (1.106)$$

Using the result from the last part, we can write $\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega)$.

$$\Rightarrow \nabla^2 \mathbf{E} = -\frac{i\omega}{c} \left(\frac{4\pi}{c} \sigma - \frac{i\omega}{c} \right) \mathbf{E} \quad (1.107)$$

$$= -\frac{\omega^2}{c^2} \left(\frac{4\pi\sigma}{\omega} + 1 \right) \mathbf{E} \quad (1.108)$$

Doing the same with the magnetic field yields:

$$-\nabla^2 \mathbf{H} = \frac{4\pi}{c} \nabla \times \mathbf{j} + \frac{\omega^2}{c^2} \mathbf{H} \quad (1.109)$$

$$= \frac{4\pi\sigma}{c} \left(-\frac{i\omega}{c} \mathbf{H} \right) + \frac{\omega^2}{c^2} \mathbf{H} \quad (1.110)$$

$$= \frac{\omega^2}{c^2} \left(1 - \frac{4\pi\sigma i}{\omega} \right) \mathbf{H} \quad (1.111)$$

Note, make sure to consider that the conductivity is a function of ω , as shown in part a).

$$\Rightarrow \nabla^2 \mathbf{E} = -\frac{\omega^2}{c^2} \left(\frac{4\pi}{\omega} \frac{\sigma_0}{1 - i(\omega \pm \omega_c)\tau} i + 1 \right) \mathbf{E} \quad (1.112)$$

Attempt 1 - Solving characteristic equation for solutions We're looking for plane waves that propagate through a particular direction, in this case z . The solutions for the electric field then follow the general solutions of the wave equation:

$$\mathbf{E} = \mathbf{E}_0 e^{\lambda z} \quad (1.113)$$

Applying the Solving coefficients:

$$\lambda^2 = -\frac{\omega^2}{c^2} \left(\frac{4\pi\sigma}{\omega} i + 1 \right) \quad (1.114)$$

$$\lambda = \pm i \frac{\omega}{c} \sqrt{\frac{4\pi\sigma}{\omega} i + 1} \quad (1.115)$$

Let $z = a + bi$, and $z^2 = \frac{4\pi\sigma}{\omega} i + 1 = (a^2 - b^2) + 2abi$. Then equating the parts,

$$a^2 - b^2 = 1 \quad (1.116)$$

$$2ab = \frac{4\pi\sigma}{\omega} \quad (1.117)$$

Calculating a:

$$\Rightarrow a^2 - \left(\frac{4\pi\sigma}{2\omega a} \right)^2 = 1 \quad (1.118)$$

$$a^4 - a^2 - \left(\frac{2\pi\sigma}{\omega} \right)^2 = 0 \quad (1.119)$$

$$\left(a^2 - \frac{1}{2} \right)^2 - \frac{1}{4} - \left(\frac{2\pi\sigma}{\omega} \right)^2 = 0 \quad (1.120)$$

$$a^2 - \frac{1}{2} = \pm \sqrt{\frac{1}{4} + \left(\frac{2\pi\sigma}{\omega} \right)^2} \quad (1.121)$$

$$a = \pm \sqrt{\frac{1}{2} \pm \sqrt{\frac{1}{4} + \left(\frac{2\pi\sigma}{\omega} \right)^2}} \quad (1.122)$$

Calculating b:

$$b = \pm \sqrt{a^2 - 1} \quad (1.123)$$

$$= \pm \sqrt{-\frac{1}{2} \pm \sqrt{\frac{1}{4} + \left(\frac{2\pi\sigma}{\omega} \right)^2}} \quad (1.124)$$

Therefore,

$$E(x, t) = E_0 e^{i(\lambda x - \omega t)} \quad (1.125)$$

$$\lambda = \pm i \frac{\omega}{c} (a + bi) \quad (1.126)$$

Attempt 2 - Verifying provided solution is valid We have been provided with the solution:

$$E_x = E_0 e^{i(kz - \omega t)}, \quad E_y = \pm i E_x, \quad E_z = 0 \quad (1.127)$$

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega} \left(\frac{1}{\omega \mp \omega_c + i/\tau} \right) \quad (1.128)$$

$$\omega_p^2 = \frac{4\pi n e^2}{m} \quad (1.129)$$

$$\omega_c = \frac{eH}{mc} \quad (1.130)$$

$$k^2 c^2 = \epsilon \omega^2 \quad (1.131)$$

Verifying this solution to the differential equation found above earlier,

$$\nabla^2 \mathbf{E} = \nabla^2 (e^{ikz - \omega t}) \mathbf{E}_0 \quad (1.132)$$

$$= i^2 k^2 \mathbf{E} \quad (1.133)$$

$$= -\frac{\omega^2}{c^2} \left(1 - \left(\frac{4\pi n e^2}{m} \right) \frac{1}{\omega \omega \mp \omega_c + i/\tau} \right) \mathbf{E} \quad (1.134)$$

$$= -\frac{\omega^2}{c^2} \left(1 - \left(\frac{4\pi n e^2}{m} \right) \frac{1}{\omega - i(\omega \mp \omega_c) \tau + 1} \right) \mathbf{E} \quad (1.135)$$

$$= -\frac{\omega^2}{c^2} \left(1 + \left(\frac{\tau n e^2}{m} \right) \frac{4\pi}{\omega} \frac{1}{-i(\omega \mp \omega_c) \tau + 1} i \right) \mathbf{E} \quad (1.136)$$

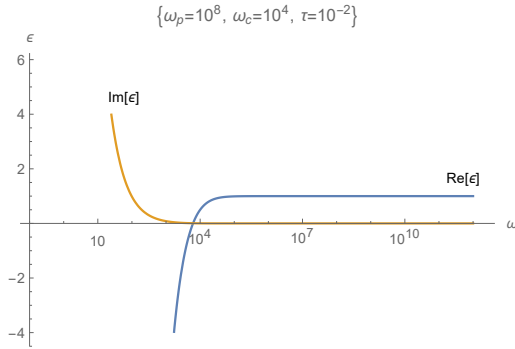
$$= -\frac{\omega^2}{c^2} \left(1 + \frac{4\pi}{\omega} \frac{\sigma_0}{1 - i(\omega \mp \omega_c) \tau} i \right) \mathbf{E} \quad (1.137)$$

which thus satisfies the result of Maxwell's equations in eq. (1.112).

1.2.4.c) Sketch of ϵ

Sketch $\epsilon(\omega)$ for $\omega > 0$ (choosing the polarisation $E_y = iE_x$) and demonstrate that solutions to $k^2 c^2 = \epsilon \omega^2$ exist for arbitrary k at frequencies $\omega > \omega_p$ and $\omega < \omega_c$. (Assume the high field condition $\omega_c \tau \gg 1$, and note that even for hundreds of kilogauss, $\omega_p/\omega_c \gg 1$.)

Plotting eq. (1.128):



Ideally the graph would demonstrate real solutions of ϵ , which correspond to real wave-vectors k . However, if there are large imaginary components of ϵ , then the wave solution has a large real exponential component, either suppressing or diverging based on sign. To demonstrate that real solutions, we first apply the assumptions to the function ($\omega_c \tau \gg 1, \omega_p/\omega_c \gg 1$).

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega} \left(\frac{1}{\omega \mp \omega_c + i/\tau} \right) \quad (1.138)$$

1.2.4.d) Estimation of Helicon frequency

Show that when $\omega \ll \omega_c$ the relation between k and ω for the low-frequency solution is

$$\omega = \omega_c \left(\frac{k^2 c^2}{\omega_p^2} \right) \quad (1.144)$$

This low-frequency wave, known as a helicon, has been observed in many metals. Estimate the helicon frequency if the wavelength is 1cm and the field is 10 kilogauss, at typical metallic densities.

$$= 1 - \frac{\omega_p^2}{\omega \omega_c} \left(\frac{1}{\omega/\omega_c \mp 1 + \frac{i}{\tau \omega_c}} \right) \quad (1.139)$$

$$= 1 - \frac{\omega_p^2}{\omega \omega_c} \left(\frac{1}{\omega/\omega_c \mp 1 + 0} \right) \quad (1.140)$$

$$= 1 - \frac{\omega_p}{\omega} \left(\frac{1}{\omega/\omega_p \mp \omega_c/\omega_p} \right) \quad (1.141)$$

$$= 1 - \frac{\omega_p}{\omega} \left(\frac{1}{\omega/\omega_p \mp 0} \right) \quad (1.142)$$

$$= 1 - \frac{\omega_p^2}{\omega^2} \quad (1.143)$$

Therefore if $\omega > \omega_p$, then the clear implications are that the term $\frac{\omega_p}{\omega}$ approaches zero. Therefore $\epsilon(\omega)$ is real and positive, thereby resulting in a complex exponent and a propagating electromagnetic field.

If $\omega < \omega_c$, then we have to consider the limit that $\frac{\omega_p}{\omega_c} \gg 1$, which then implies $\frac{\omega_p}{\omega} \gg 1$. In this case $\epsilon(\omega)$ is also real but negative, thereby also resulting in a complex exponent and a propagating electromagnetic field.

Low Frequency Solution Starting with the condition from part b),

$$\omega \left(\frac{\omega_p^2}{\omega_c} \right) = k^2 c^2 \quad (1.149)$$

$$\omega^2 \epsilon(\omega) = k^2 c^2 \quad (1.145)$$

$$\omega = \omega_c \left(\frac{k^2 c^2}{\omega_p^2} \right) \quad (1.150)$$

Estimation

$$\omega^2 \left(1 - \frac{\omega_p^2}{\omega} \left(\frac{1}{\omega \mp \omega_c + i/\tau} \right) \right) = k^2 c^2 \quad (1.146)$$

$$\omega = \omega_c \left(\frac{k^2 c^2}{\omega_p^2} \right) \quad (1.151)$$

$$\omega^2 \left(1 - \omega_p^2 \left(\frac{\frac{1}{\omega_c}}{\frac{\omega^2}{\omega_c} \mp \frac{\omega_c \omega}{\omega_c} + i \frac{\omega}{\tau \omega_c}} \right) \right) = k^2 c^2 \quad (1.147)$$

$$\omega_p = \frac{4\pi n e^2}{m_e} \quad (1.152)$$

$$\omega_c = \frac{eH}{m_e c} \quad (1.153)$$

When $\omega \ll \omega_c$,

$$\omega^2 \left(1 - \omega_p^2 \left(\frac{1/\omega_c}{\mp \omega} \right) \right) = k^2 c^2 \quad (1.148)$$

Assuming $\omega_p \gg \omega_c$ as reasoned in part c).

Using typical free-electron metallic densities of $1 \times 10^{22} \text{ cm}^{-3}$, and inferring the wavevector $k = c/\lambda$, we get

$$\omega = \frac{Hc}{2ne\lambda^2} = 308 \text{ Hz} \quad (1.154)$$

1.2.5 Surface Plasmons

An electromagnetic wave that can propagate along the surface of a metal complicates the observation of ordinary (bulk) plasmons. Let the metal be contained in the half space $z > 0$, $z < 0$ being vacuum. Assume that the electric charge density ρ appearing in Maxwell's equations vanishes both inside and outside the metal. (This does not preclude a surface charge density concentrated in the plane $z=0$.) The surface plasmon is a solution to Maxwell's equations of the form

$$E_x = A e^{iqx - Kz} \quad E_y = 0, \quad E_z = B e^{iqx - Kz}, \quad z > 0; \quad (1.155)$$

$$E_x = C e^{iqx - K'z} \quad E_y = 0, \quad E_z = D e^{iqx - K'z}, \quad z < 0; \quad (1.156)$$

$$\{q, K, K'\} \in \mathbb{R}, \quad \{K, K'\} > 0 \quad (1.157)$$

1.2.5.a) Relate q , K and K'

Assuming the usual boundary conditions, (\mathbf{E}_{\parallel} continuous, $(\epsilon \mathbf{E})_{\perp}$ continuous), and using the Drude results (1.35) and (1.29) find three equations relating q , K , and K' as functions of ω .

We have 7 unknowns, however the relative amplitude can remain unsolved, so 6 unknowns. Hence we need to have 6 equations to solve for all variables. This can be done by using 2 equations at the interface (in-plane and out-of-plane), and using the wave equation and divergence equations on the 4 provided fields in the question.

Note, the Drude results are

$$\epsilon(\omega) = 1 + \frac{4\pi\sigma}{\omega} i \quad (1.158)$$

$$\sigma(\omega) = \left(\frac{ne^2\tau}{m_e} \right) \frac{1}{1 - i\omega\tau} \quad (1.159)$$

Boundary Conditions Using usual boundary conditions (ie Gauss' law), and ϵ as per the Drude result in the metal. **The reason for the perpendicular (to the interface) direction to include ϵ is that it originates from Gauss' law, and only observed the bound charge inside, which is related to the difference in ϵ . Parallel to the interface directions require no ϵ because as you shrink the proximity**

of a surface loop, there can be no discontinuity between fields.

$$\{\mathbf{E}_{\parallel z+} = \mathbf{E}_{\parallel z-}\}_{|z=0} \quad (1.160)$$

$$\{\epsilon(\omega)\mathbf{E}_{\perp z+} = \mathbf{E}_{\perp z-}\}_{|z=0} \quad (1.161)$$

Considering amplitude at $z=0$, the \mathbf{E}_{\perp} case:

$$\Rightarrow \epsilon(\omega)Be^{iqx} = De^{iqx} \quad (1.162)$$

$$\frac{D}{B} = \epsilon(\omega) \quad (1.163)$$

and the \mathbf{E}_{\parallel} case:

$$\Rightarrow Ae^{iqx} - Ce^{iqx} = 0 \quad (1.164)$$

$$\rightarrow A \equiv C \quad (1.165)$$

Divergence It is appropriate to use Gauss' law, where there is no charge density in the mediums

$$\nabla \cdot \mathbf{E} = 0 \quad (1.166)$$

Applying to the metal side $z > 0$

$$iqAe^{iqx-Kz} - KB e^{iqx-Kz} = 0 \quad (1.167)$$

$$iqA - KB = 0 \quad (1.168)$$

and likewise in the vacuum,

$$iqCe^{iqx+K'z} + K'De^{iqx+Kz} = 0 \quad (1.169)$$

$$iqC + K'D = 0 \quad (1.170)$$

Wave equation For the Drude metal;

$$\nabla^2 \mathbf{E} = -\frac{\omega^2}{c^2} \left(\frac{4\pi\sigma(\omega)}{c} \mathbf{i} + 1 \right) \mathbf{E} \quad (1.171)$$

Applying this to the metal $z > 0$,

$$\nabla^2 \mathbf{E} = \nabla^2 e^{iqx-Kz} \begin{bmatrix} A \\ B \end{bmatrix} \quad (1.172)$$

$$= (iq)^2 + (-K)^2 e^{iqx-Kz} \begin{bmatrix} A \\ B \end{bmatrix} \quad (1.173)$$

$$= (-q^2 + K^2) \mathbf{E} \quad (1.174)$$

Equating to the wave equation, we have:

$$(-q^2 + K^2) = -\frac{\omega^2}{c^2} \left(\frac{4\pi\sigma(\omega)}{c} \mathbf{i} + 1 \right) \quad (1.175)$$

Likewise for the vacuum,

$$\nabla^2 \mathbf{E} = ((iq)^2 + (K')^2) \mathbf{E} \quad (1.176)$$

$$= (-q^2 + K'^2) \mathbf{E} \quad (1.177)$$

However, the wave equation differs, as $\mathbf{j} = 0$

$$\nabla^2 \mathbf{E} = -\frac{\omega^2}{c^2} \mathbf{E} \quad (1.178)$$

Therefore equating we find

$$(-q^2 + K'^2) = -\frac{\omega^2}{c^2} \quad (1.179)$$

Combining the equations Summarising the results we had:

$$A = C \quad (1.180)$$

$$D = \epsilon(\omega)B \quad (1.181)$$

$$iqA = KB \quad (1.182)$$

$$iqC = -K'D \quad (1.183)$$

$$(-q^2 + K^2) = -\frac{\omega^2}{c^2} \epsilon(\omega) \quad (1.184)$$

$$(-q^2 + K'^2) = -\frac{\omega^2}{c^2} \quad (1.185)$$

Solving these equations by using the last four equations in the summary,

$$K^2 - K'^2 = \frac{\omega^2}{c^2} (1 - \epsilon(\omega)) \quad (1.186)$$

$$\frac{K}{K'} = -\frac{iqAD}{iqBC} \quad (1.187)$$

Using the first two equations in the summary,

$$\frac{iqAD}{iqBC} = \epsilon(\omega) \quad (1.188)$$

$$\Rightarrow \frac{K}{K'} = -\epsilon(\omega) \quad (1.189)$$

Substituting K' :

$$K^2 - \left(\frac{K}{\epsilon(\omega)} \right)^2 = \frac{\omega^2}{c^2} (1 - \epsilon(\omega)) \quad (1.190)$$

$$K^2 \left(1 - \frac{1}{\epsilon(\omega)^2} \right) = \frac{\omega^2}{c^2} (1 - \epsilon(\omega)) \quad (1.191)$$

$$K^2 = \frac{\omega^2}{c^2} \times \frac{\epsilon(\omega)^2 (1 - \epsilon(\omega))}{\epsilon(\omega)^2 - 1} \quad (1.192)$$

$$K^2 = -\frac{\omega^2}{c^2} \frac{\epsilon(\omega)^2}{\epsilon(\omega) + 1} \quad (1.193)$$

$$K = \pm \frac{\omega \epsilon(\omega)}{c \sqrt{\epsilon(\omega) + 1}} \mathbf{i} \quad (1.194)$$

Therefore applying to K' ,

$$K' = \mp \frac{\omega}{c\sqrt{\epsilon(\omega)+1}}i \quad (1.195)$$

and finally q :

$$q^2 = K^2 + \frac{\omega^2}{c^2}\epsilon(\omega) \quad (1.196)$$

$$= -\frac{\omega^2}{c^2} \frac{\epsilon(\omega)^2}{\epsilon(\omega)+1} + \frac{\omega^2}{c^2}\epsilon(\omega) \quad (1.197)$$

$$= \frac{\omega^2}{c^2} \frac{\epsilon(\omega)(\epsilon(\omega)+1)}{\epsilon(\omega)+1} - \frac{\omega^2}{c^2} \frac{\epsilon(\omega)^2}{\epsilon(\omega)+1} \quad (1.198)$$

$$= \frac{\omega^2}{c^2} \frac{\epsilon(\omega)}{\epsilon(\omega)+1} \quad (1.199)$$

1.2.5.b) Plot

Assuming that $\omega\tau \gg 1$, plot q^2c^2 as a function of ω^2 .

By assuming $\omega\tau \gg 1$ we're neglecting the imaginary part of ϵ :

$$\epsilon(\omega) = 1 + \frac{4\pi}{\omega} \left(\frac{1}{1-i\omega\tau} \right) \left(\frac{ne^2\tau}{m_e} \right) i \quad (1.200)$$

Use approximation, $\omega\tau \gg 1$

$$= 1 + \frac{4\pi}{\omega} \left(\frac{1}{-i\omega\tau} \right) \left(\frac{ne^2\tau}{m_e} \right) i \quad (1.201)$$

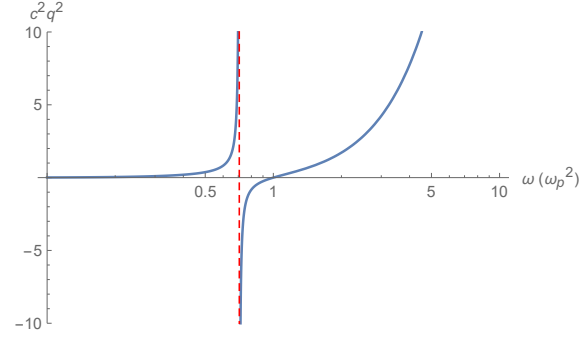
$$= 1 - \frac{1}{\omega^2} \left(\frac{4\pi ne^2}{m_e} \right) = 1 - \frac{\omega_p^2}{\omega^2} \quad (1.202)$$

Therefore,

$$q^2c^2 = \omega^2 \frac{\epsilon(\omega)}{\epsilon(\omega)+1} \quad (1.203)$$

$$= \omega^2 \left(1 - \frac{1}{\epsilon(\omega)+1} \right) \quad (1.204)$$

$$= \omega^2 \left(1 - \frac{1}{2 - \frac{\omega_p^2}{\omega^2}} \right) \quad (1.205)$$



1.2.5.c) The surface plasmon

In the limit as $qc \gg 1$, show that there is a solution at the frequency $\omega = \omega_p/\sqrt{2}$. Show from an examination of K and K' that the wave is confined to the surface. Describe its polarisation. This wave is known as a surface plasmon.

If $\omega = \omega_p/\sqrt{2}$, we can evaluate the original solution to determine the nature of the wave and its polarisation. Note what the limit $qc \gg \omega$ implies:

$$q^2c^2 \gg \omega^2 \quad (1.206)$$

$$\Rightarrow q^2c^2 = \omega^2 \frac{\epsilon(\omega)}{\epsilon(\omega)+1} \gg \omega^2 \quad (1.207)$$

$$\rightarrow \frac{\epsilon(\omega)}{\epsilon(\omega)+1} \gg 1 \quad (1.208)$$

Therefore as q is the coefficient for the speed of propagation in the x axis, the solution both in the vacuum and the metal oscillate fast relative

to the frequency ω . Evaluating $\epsilon(\omega)$:

$$\epsilon(\omega) = 1 + \frac{4\pi}{\omega} \left(\frac{1}{1-i\omega\tau} \right) \left(\frac{ne^2\tau}{m_e} \right) i \quad (1.209)$$

$$= 1 + \frac{1}{\omega} \left(\frac{\tau}{1-i\omega\tau} \right) \left(\frac{4\pi ne^2}{m_e} \right) i \quad (1.210)$$

$$= 1 + \frac{1}{\omega} \left(\frac{\tau}{1-i\omega\tau} \right) (\omega_p^2) i \quad (1.211)$$

$$= 1 + \frac{\tau\omega_p^2}{\omega(1-i\omega\tau)} i \quad (1.212)$$

Multiply num. and den. by conjugate.

$$= 1 + \frac{\tau\omega_p^2}{\omega(1+\omega^2\tau^2)} (i-\omega\tau) \quad (1.213)$$

$$= 1 - \frac{\tau^2 \omega_p^2}{1 + \omega^2 \tau^2} + \frac{\tau \omega_p^2}{\omega (1 + \omega^2 \tau^2)} i \quad (1.214)$$

Still assuming conditions $\omega \tau \gg 1, \omega > \tau$

$$\approx 1 - \frac{\omega_p^2}{\omega^2} \quad (1.215)$$

And evaluating q with $\omega \rightarrow \omega_p/\sqrt{2}$:

$$q^2 = \frac{\omega^2}{c^2} \frac{\epsilon(\omega)}{\epsilon(\omega) + 1} \quad (1.216)$$

$$q^2 = \frac{\omega^2}{c^2} \left(\frac{1 - \omega_p^2/\omega^2}{2 - \omega_p^2/\omega^2} \right) \quad (1.217)$$

$$= - \lim_{\omega \rightarrow \omega_p/\sqrt{2}} \left[\frac{\omega^2}{c^2 (2 - \omega_p^2/\omega^2)} \right] \quad (1.218)$$

$$q = \pm \lim_{\omega \rightarrow \omega_p/\sqrt{2}} \left[\frac{\omega^2}{c \sqrt{2\omega^2 - \omega_p^2}} i \right] \quad (1.219)$$

$$(1.220)$$

Considering K',

$$K' = \mp \frac{\omega}{c \sqrt{\epsilon(\omega) + 1}} i \quad (1.221)$$

$$= \mp \frac{\omega^2}{c \sqrt{2\omega^2 - \omega_p^2}} i \quad (1.222)$$

Considering K:

$$K = \pm \frac{\omega \epsilon(\omega)}{c \sqrt{\epsilon(\omega) + 1}} i \quad (1.223)$$

$$= \pm \frac{\omega^2}{c \sqrt{2\omega^2 - \omega_p^2}} \left(1 - \frac{\omega_p^2}{\omega^2} \right) i \quad (1.224)$$

$$= \mp \lim_{\omega \rightarrow \omega_p/\sqrt{2}} \frac{\omega^2}{c \sqrt{2\omega^2 - \omega_p^2}} i \quad (1.225)$$

$$(1.226)$$

K has the same as the signed decay rate as K'. This is also the same as q. Therefore

$$\lim_{\omega \rightarrow \omega_p/\sqrt{2}} \{K' \cong K\} = q \quad (1.227)$$

Having confirmed the exponential components, consider the relation of coefficients between X and Z directions. A,B,C,D to check the polarisation. From part a),

$$iqA = KB \quad (1.228)$$

$$iqC = -K'D \quad (1.229)$$

Using the relations for K, K' and q found above,

$$iA = B \quad (1.230)$$

$$iC = -D \quad (1.231)$$

Clearly the denominator diverges as $\omega \rightarrow \omega_p/\sqrt{2}$, implying that moving away from $z = 0$ causes a large suppression in the plasmon amplitude.

This is the exact case of 90° phase between E_x and E_z components, meaning circularly polarised light.

Chapter 2

The Sommerfeld Theory of Metals

2.1

It was assumed for many years during and after Drude's time that the distribution of velocities were given by the Maxwell-Boltzmann distribution, just like ideal gasses.

Free electron approximation: However, now assuming that there are just free electrons, and that interaction between valence electrons and ions are neglected, except in boundary conditions. Ions not necessarily the source of collisions. Why is this significant?

- Pauli Exclusion
- Fermi Dirac distribution
- Particle in a box
- Particle in a box with open boundaries
- Energies of a particle in a box, similarity to that of free classical forms
- De-broglie wavelength
- Applying boundary conditions to discretize wavevector values. Is

$$e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1 \quad (2.1)$$

really the only solution? YES

- Approximation of number of allowed states (Fermi Sphere)
- Typical values of k-space in materials Each wavevector \mathbf{k} has two spin states. Allowed number of states of \mathbf{k} within a sphere is

- General quantities, evaluation to conduction electron density.
- "Unimaginative" Nomenclature lmao
- Velocity, statistical mechanics. 1% of light. At $T=0$, ground state.
- Ryberg, A_0 and r_S .
- Fermi Energies
- Ground state energy & approximation of summation to that of an integral.
- Energy per electron.
- Measurements of Bulk Moduli to confirm pressure calculation

2.1.1 Stat mech of thermal properties

- Non-zero temp, need to use the partition function to acknowledge the weight of each state.
- Helmholtz free energy from statistical mechanics
- Probability of an electron being in energy level i given thermal equilibrium.
- Assumption that at large N , the probability of a being in level i is roughly the same as if $N \rightarrow N+1$.
- Chemical potential distinguished from Fermi energy
- Heat capacity and density of levels per unit volume
 - In general $T < T_f$.
 - Sommerfeld expansion
 - Mathematical magic to get rid of integral term from μ to ∞ . (2.70)
 - Apply expansion to electronic energy u and number density n ($C_v = \left. \frac{du}{dT} \right|_V, u = \frac{U}{V}, n = \frac{N}{V}$)
 - Resolve the fact that the number density is independent of temperature to solve for the chemical potential.
 - Cancel term in the energy density.
 - Solve heat capacity.

Observations: The values of this specific heat are suppressed by factor 10^{-2} compared to that of the classical result.

"This explains lack of observation of electronic degrees of freedom to specific heat at room temp" - This is simply just saying that as a result of the electronics (ideal gas behaviour) shows little contribution.

Understanding of the model - how the Fermi function shows that as T increases from 0, some electrons can now be excited by temperature, so the distribution is no longer a step. The width $k_B T$ becomes very important, considered with the density of energy levels per unit volume at that Fermi-energy. The excitation energy is also roughly the width, and so you can estimate the thermal energy density, as the excitation energy multiplied by the density of energy levels per unit volume at the Fermi-energy. It's only out by factor 1.8.

This has been not been good for predicting high temperature situations, as specific heat is dominated by ionic degrees of freedom at high temperature. Not so the case at low temperature. Linear term can be measured when the contribution becomes equivalent, confirming the prediction of Fermi-Dirac statistics.

Some massive exceptions experimentally in Mn, Bi and Sb. (All magnetic heavy metal elements?).

2.1.2 Conduction Theory

- Velocity in metals derived using Pauli exclusion to find a velocity element and Fermi-Dirac distributions of velocities
- Sommerfeld substituted Maxwell-Boltzmann for Fermi-Dirac, but why only affect the statistics, and not the dynamics?
- Uncertainty principle implies that classical descriptions only possible if $\Delta x \gg r_s$, ie bound within atomic distances.
- Positions of electrons considered in Drude model?
 - Fields or gradients, specify position of electron on a small scale compared to scale of the field λ .
 - Localisation can occur to within less than a mean free path ℓ . Be suspicious of classical arguments for paths less than 10 Å. In metals, this is fine, $\ell \approx 100$ Å.
- Reintroduce electromagnetic field to non-interacting electrons.
- Behaviour can be determined by N non-interacting independent one-electron problems...
- If collision rate is unchanged, then estimates of electronic mean free path, thermal conductivity and thermopower are all affected by a change in equilibrium function.

2.1.3 Applications of Fermi-Dirac distribution

Chapter 3

Quantum Transport

3.1 Introduction

Background includes a channel between a source and a drain. The conduction is dependent upon the amount of modes / states within that channel.

There are mechanical force driven and entropy driven mechanisms.

To combine both of these mechanisms for semi-classical transport, it took a bit of effort,

into something called "Boltzmann" dynamics. It combines Newton mechanics, and entropy.

In quantum transport, we now have wave nature of electrons, plus the entropy, to be able to get NEGF. We'll have a Schrödinger equation to be able to generate a Hamiltonian of whose eigenvalues specify the energy levels.

3.1.1 Energy of an atom

$$E = -\frac{Zq^2}{4\pi\epsilon_0 r} + \frac{mv^2}{2} = -\frac{Zq^2}{8\pi\epsilon_0 r} \quad (3.1)$$

When we looked at the spectra of atoms, hydrogen, we found that very particular colours came from that light. Specific frequencies, with specific energy differences.

In about 1915, they said that electrons are waves, and that it's pathlength / circumference must be a multiple of the wavelength (de Broglie). This gives you allowed values of r from now. Only specific values will fit. This is the Bohr radius. It's about 0.5Å or 1/20th of a nanometer.

$$r_n = \frac{4\pi\epsilon_0 \hbar^2}{mq^2} \times \frac{n^2}{Z} \quad (3.2)$$

To put this into a solid mathematical footing, we have the Schrödinger equation guessed.

$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \psi(\vec{r}) \quad (3.3)$$

Particular functions will make this equation work, and there would be a resultant specific energy. The other thing that was realised is that you could write multiple wave functions that would give the same energy. Multiple levels having the same energy. This occurred with the **s** and **p** electron levels.

This was then applied to almost all atoms in the periodic table. As you grow a larger nucleus with a larger positive charge, you find that the energy levels go deeper and deeper. You can measure these

experimentally, through the use of photo emission (energy level transition & photoelectric effect). Experiment and theory are in good agreement.

As soon as you go from hydrogen to helium, then the potential becomes much much more complex - because of the electron electron interactions. They try to push each other out. They did do it by 1960, which is pretty cool.

We're interested in periodic solids. These are quite different. The common method to solve the Schrödinger equation is the use of "basis functions" to convert a differential equation into a matrix equation.

$$\psi(\vec{r}) = \sum_{m=1}^N \psi_m \mu_m(\vec{r}) \quad (3.4)$$

So we write it as some number of each of the functions of individual atoms, a linear combination. We can use powerful methods to find the eigenvalues of the complex matrices that have these properties.

Two methods for these calculations

- **First principles.** Uses Gaussian basis functions. There would be a function for every atom, your basis would be N dimensional.
- **Semi-empirical method.** Use a few basic parameters from known experiments, then use these to generate much more complex models. How to compare to experiment. We'll be using this part of the story. The "band structure of a solid".

3.1.2 Wave equation

Differential equations are difficult to solve. You can always check a solution is right or not though. Lets simplify the Schrödinger equation for a little bit to solve it, by using a constant potential.

$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U_0 \right) \psi(\vec{r}) \quad (3.5)$$

We can easily write down a solution to this, in terms of plane waves. A solution for this equation is simply

$$\psi(\vec{r}) = e^{ik_x x} e^{ik_y y} e^{ik_z z} \psi_0 = e^{i\vec{k} \cdot \vec{r}} \quad (3.6)$$

Plugging this in solves the equation by producing a dispersion relationship:

$$E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) + U_0 \quad (3.7)$$

3.1.2.1 Particle in a box

A simple example of such a use of the Schrödinger equation is the particle in a box situation, where the U_0 is constant at particular locations. However for this situation, we actually need two solutions rather than just a single sign of the exponential.

$$\psi(z) = Ae^{ik_z z} + Be^{-ik_z z} \quad (3.8)$$

When you solve this, you get a sinusoidal function, but you also need to impose a restriction on the values of k_z to ensure it meets the box walls / edges. So it becomes quantised. Consequentially

you can see how the energies also become discretised. Note also $\psi\psi^*$ is the chance of finding a single electron. However, when you're talking about a system of many many electrons, then we're talking more likely about an electronic density.

Confined waves have resonance. Classical example? Guitar string pinned by two ends.

3.1.2.2 Crystals

In crystals, we have two situations - areas of a material where there's very discretized states, called the "core" states. But additionally to this are the more continuous states where electrons are spread out through the material.

$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m_0} \nabla^2 + U(\vec{r}) \right) \psi(\vec{r}) \quad (3.9)$$

Here m_0 is the free electron mass.

Such a regime is quite unique - electrons experience a periodic potential, and this manifests itself in the behaviour of the electron as if it was in a vacuum, but now with a different effective mass. And so we have a new wave equation:

$$E\psi(\vec{r}) = \left(-\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}) \right) \psi(\vec{r}) \quad (3.10)$$

Here you don't need to put in the atomic potentials. So if you do include a potential term, it's actually describing

Chapter 4

Bibliography