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Plasmons in Topological Insolators

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Contents

Dedicated to my parents.

1. Prologue

1.1. Structure of this thesis

This thesis is divided into five chapters plus appendix. Without further ado, we outline the basic formalism and concepts needed to describe plasmons and introduce topological insulators in chapter two.
In chapter number three we model plasmons in topological insulators and develop our formalism to include effects of a topological term. Furthermore, all the main calculations of this work are carried out in this chapter.
The results, including their discussion are subject to chapter four.
A recapitulation can be found in the last chapter, summarizing the workflow and the final results.

1.2. Measurement units

We use SI units throughout. During the explicit calculation of the polarization function of free massless Dirac electrons, we will set $v_F = \hbar = 1$, so that $\mu = k_F$. The quantities plotted in the figures are almost exclusively expressed in Hertz [Hz] and inverse meter $[m^{-1}]$, alternatively in units of $\frac{\mu}{\hbar^2 v_F^2}$.
Depending on the typical notation for each subject, k_x and q are used synonymously in this thesis.

2. Basics/Theory

In this chapter we start with a very short review of the basic equations of electrodynamics in section 2.1.
In section 2.2 we give a brief and not very technical introduction to topological insulators - for a more sophisticated overview of this interesting subject we refer to review articles given in the appendix.
In 2.3 we derive the "ordinary" plasmon condition on an interface between two dielectrics before introducing the concept of the dielectric function in the random phase approximation in section 2.4, which marks the initial point for our calculation of the polarization function of free massless Dirac electrons in chapter 3.

2.1. Maxwell's Equations

The foundation of classical electrodynamics is built on a set of partial differential equations, known as Maxwell's equations, that describe how electric and magnetic fields are generated and influenced by each other and by electrical charges and currents.

Macroscopic Maxwell equations in SI units

$$\vec{\nabla} \cdot \vec{D} = \rho, \qquad \text{(Gauss's Law)} \tag{2.1a}$$

$$\vec{\nabla} \cdot \vec{B} = 0, \qquad \text{(magnetic analogon)} \tag{2.1b}$$

$$\vec{\nabla} \times \vec{H} = \vec{\jmath} + \frac{\partial \vec{D}}{\partial t}, \qquad \text{(Ampère's Circuital Law with Maxwell's correction)} \tag{2.1c}$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}. \qquad \text{(Faraday's Induction Law)} \tag{2.1d}$$

$\vec{D}$ describes the electric displacement field, $\vec{E}$ the electric field, $\vec{B}$ the magnetic induction and $\vec{H}$ the magnetic field, ρ the free charge density and $\vec{\jmath}$ the free current density.

Gauss's Law (2.1a), respectively Gauss's flux theorem, states, that the electric flux through any hypothetical closed surface is proportional to the enclosed electric charge, or in other words: electrical charges are the sources of the electric field.

Its magnetic analog (2.1b) on the other hand postulates that no magnetic monopoles exist.

Ampère's Circuital Law with Maxwell's correction (2.1c) describes in its original form (without the correction term including the time derivative of the electrical displacement field $\vec{D}$) the relation between electric currents and the magnetic fields they produce. As can be seen from the occurrence of the time derivative in (2.1c), Ampère's original Circuital Law is correct only in a magnetostatic situation. In all other situations the displacement current (which is not an electric current made of moving charges, but a variation in time of an electric field) has to be added, as it produces its own magnetic field, just as currents do.

Finally, Faraday's Induction Law (2.1d) connects time variation of the magnetic induction $\vec{B}$ with an electric field it induces - the basic operating principle behind electric generators.

Implicit in Maxwell's equations is the continuity equation relating timely changes in the electric charge density ρ to spatial changes of the electric current density $\vec{j}$:

Continunity Equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0 \tag{2.2}$$

Last but not least, before doing calculations in electrodynamics, it is necessary to specify relations between displacement field $\vec{D}$ and electric field $\vec{E}$ as well as between the magnetic field $\vec{H}$ and the magnetic induction $\vec{B}$. These equations are know as constitutive relations and define the response of bound charge and current to the applied fields.

Constitutive Relations

$$\vec{D} = \epsilon_0 \epsilon_r \vec{E} \tag{2.3a}$$

$$\vec{H} = \frac{\vec{B}}{\mu_0 \mu_r} \tag{2.3b}$$

ϵ_r is the relative permittivity, ϵ_0 the permittivity of free space, μ_r the relative permeability and μ_0 the permeability of free space. [15]

2.2. Topological Insulators

In this chapter we give a brief phenomenological introduction to the interesting subject of topological insulators. For a more sophisticated overview we refer to [9,20,23]. We start with a short presentation of phases of matter in section 2.1.1, where we illustrate the constraints of the description of states of matter via Landau symmetry-breaking, thereby motivating the concept of topological order which is presented in section 2.1.2. In 2.1.3, the slightly different symmetry protected topological order will be described with its prominent example, the topological insulator, which is the subject of section 2.1.4. We conclude this short introduction to topological insulators with the topological magneto electric effect in 2.1.5.

2.2.1. Phases of Matter

In everyday life, the four states of matter observed are basically solid, liquid, gas and plasma. Anyway, there exist several other, more "exotic" states, that gain a lot of interest in physics, like Bose-Einstein condensates at the very low energy scale [2], or the (possible) quark-gluon plasma at very high energies [3]. Without listing and describing all known, respectively predicted states - which is an interesting subject in its own - we want to focus on the description and classification of phase transitions and reveal the necessity of a new kind of parameter to distinguish between different phases of matter. Different *phases* may be described as different *states* of matter, but in a certain *state* of matter, there might also exist distinct *phases*. For example the melting of ice is a phase transition, that also changes the state of matter, whereas the transition from ordered magnetic moments of a ferromagnet to disordered and the accompanying "demagnetization" at the Curie temperature, changes the phase, but not the materials state. [6]

Even a remotely appropriate discussion of phase transitions would exceed the dimension of this whole thesis by far, we will therefore just list some major concepts and ideas without making any claim to be exhaustive.

Historically, states of matter were distinguished based on qualitative differences in properties. Solids were described as being fixed in volume and shape. Liquids also share a fixed volume, but have a variable shape and finally gas has no fixed volume nor shape.

In a more sophisticated approach, different phases of matter can be understood with the concept of spontaneous symmetry breaking. [24] For example freezing water, changing its phase (and state) from liquid to solid, loses its continuous translational symmetry. A magnet, having a north and south pole, gains rotational symmetry when heated above the Curie temperature.

The concept of spontaneous symmetry breaking can be visualized with a Mexican hat potential. [7] We imagine the rotational symmetry of a ferromagnet above the Curie temperature being symbolized by the symmetric potential on the left side of figure 2.1. Cooling down the "magnet", the magnetic moments become orientated, symbolized by the ball rolling one way - the final result is a symmetry broken state.

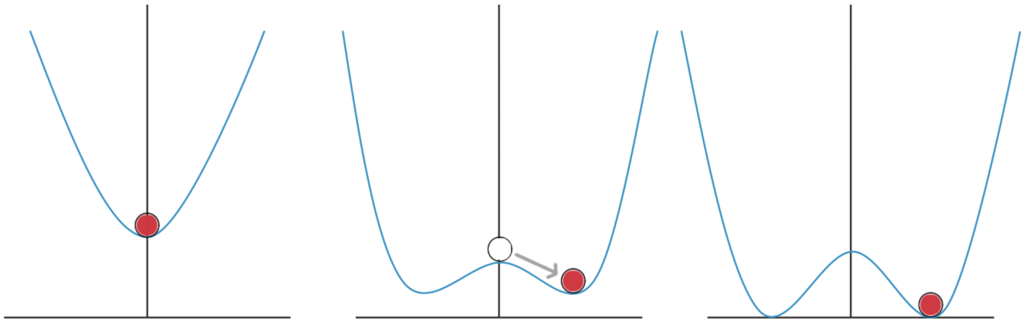

Figure 2.1.: Simplified model of spontaneous symmetry breaking in form of a Mexican hat potential: The ball is initially located at the minimum at the center in a high energy state (left). Even though the potential on the right is still symmetrical, the "local" symmetry is broken as the ball must (randomly) roll one way or the other.

2.2.2. Topological Order

The concept of spontaneous symmetry breaking, as mentioned in the previous section, reaches its limits, when trying to describe phase transitions in zero temperature phase of matter. This was first observed in high temperature superconductivity, where the chiral spin state was introduced in an (eventually abortive) effort, to find a theoretical description. [16,29] According to Landau's symmetry breaking, this new state could be understood as a state that breaks the time reversal and parity symmetries, but not the spin rotation symmetry. However, there exist many different chiral spin states with exactly the same symmetry, so Landau's symmetry breaking description does not suffice to distinguish between different chiral spin states. [25] Therefore, a new kind of order, called topological order, respectively intrinsic topological order, has to be established to distinguish between different phases in zero temperature phase of matter. [26]
The theory of topological order also allows to distinguish between different quantum Hall states that all have the same symmetry. [28]

Topological orders are described by a new set of quantum numbers like ground state degeneracy, quasiparticle fractional statistics, edge states, etc., that emerge from different patterns of long range entanglements and can not change into each other without a phase transition. A special property of topologically ordered states is the occurrence of non-trivial boundary states, leading to potential applications in electronic devices. [27]

2.2.3. Symmetry Protected Topological Order

Before we cover topological insulators, that also have gapless boundary states similar to topological order [17, 21], in the next section, we have to discuss symmetry protected topological order. In fact, topological insulators are an example of symmetry protected topological order, as they only have short-ranged entanglements. [4]
Short range entangled states all belong to one phase, but in the presence of symmetry, they can belong to different phases. Those phases therefore contain symmetry protected topological order.

If the symmetry at the boundary of symmetry protected topological order is not spontaneously broken, there are always protected gapless boundary excitations. Even if the sample is cut to form the boundary, this boundary excitations remain gapless as long as the symmetry is not broken at the boundary. In contrast to the gapless boundary excitations that may exist at intrinsic topological order, that are robust against any local perturbations, the gapless boundary excitations in symmetry protected topological order are only robust against non symmetry breaking local perturbations. Hence we find topological protected gapless boundary excitations in intrinsic topological order and symmetry protected gapless boundary excitations in symmetry protected topological order. [8, 22]

2.2.4. Topological Insulators

Prior to describing topological insulators, let's quickly recall the major statements of the previous sections:

Phase transitions can by understood via the Landau symmetry-breaking theory. In order to describe phases in highly entangled quantum matter, we need new concepts, found in topological order for long range entangled sates and symmetry protected topological order for short range entangled states in the presence of symmetry.

A topological insulator as a prominent example for latter. It is a material, that is an insulator in its interior, but whose surface contains conducting states. [18]
Looking at an idealized band structure for a topological insulator (figure 2.2), we find the electronic structure of an ordinary band insulator, with the Fermi level between conduction and valence bands in its bulk. Beyond that, there are special states on its surface that fall within the bulk energy gap. These states allow for metallic conduction and have their spin locked at a right-angle to their momentum. The surface states are a consequence of time-reversal symmetry and the band structure and can not be removed by non time-reversal symmetry breaking perturbations.

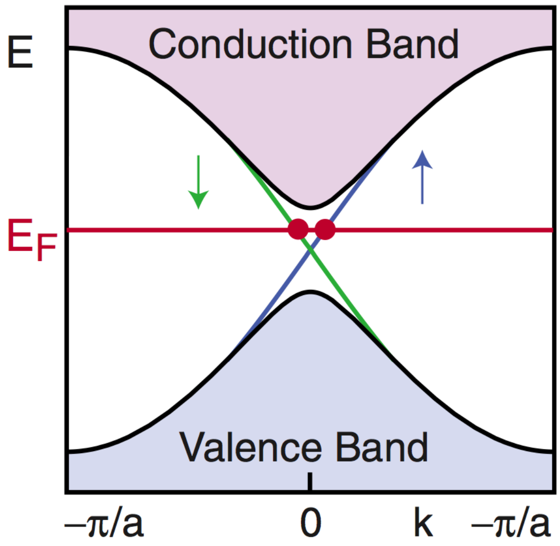

Figure 2.2.: Idealized band structure for a topological insulator with the Fermi energy within the bulk's band gap and the dispersion relation of the edge states with up and down spins. [9]

An important distinction between these topological surface states and those in the Quantum Hall effect is the locking of spin and momentum in the former ones. The characteristic of topological insulators lies in the existence of a gas of helical Diarc fermions, that has been observed in 3D topological insulators. [23]
The first experimentally observed surface states in 3D topological insulators were found using ARPES in bismuth antimonide and followed later by the discoveries in pure antimony, bismuth selenide, bismuth telluride and antimony telluride. [5,11,12,32,33]

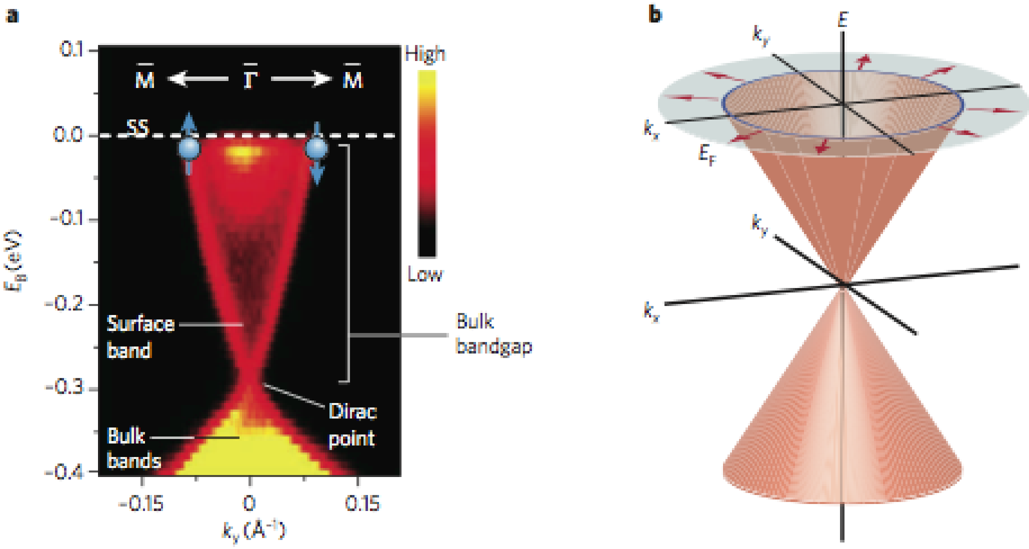

Figure 2.3.: **a)** Densityplot of the electronic structure of Bi_2Se_3, measured with ARPES, and **b)** its theoretical idealization. [20]

2.2.5. TME-Effect

A magnetization induced by an electric field, or alternatively, a charge polarization induced by a magnetic field, is defined as a magneto-electric effect. In this section, we outline the derivation of modified constituent equations for a topological insulator, describing its response to electromagnetic fields.

When TR symmetry is broken on the surface, but not in the bulk, of a 3D topological insulator, the quantized electromagnetic response turns out to be a TME effect. In this section we present a physically intuitive explanation and leave a rigorous derivation to relevant literature.

In figure 2.4, the relation between the topological magneto electric effect and the surface half Quantum-Hall effect is shown.

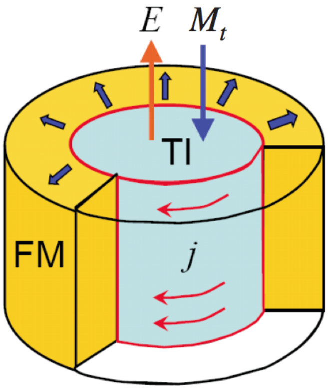

Figure 2.4.: The topological magneto electric effect and its relation to the surface QH effect. A magnetization is induced by an electric field due to a surface Hall current. [23]

The sides of the topological insulator are covered by ferromagnetic impurities in order to gap the surface states. An electric field $\vec{E}$ applied parallel to the surface induces a Hall current $\vec{\jmath}$ which circulates along the surface, perpendicular to $\vec{E}$. A magnetic field, parallel to $\vec{E}$ will then be induced by this current, so that we see an magneto electric response. This can be described with the Hall response equation

Hall Response Equation

$$\vec{\jmath} = \frac{m}{|m|}\frac{e^2}{2h}\vec{n} \times \vec{E}, \tag{2.4}$$

where $\vec{n}$ is the unit vector normal to the surface, e the electric charge, h the Planck constant, m the mass and its sign $\frac{m}{|m|}$ determined by the direction of the surface magnetization. This Hall response is equivalent to a magnetization of the form

Hall Response Equivalent Magnetization

$$\vec{M}_t = -\frac{m}{|m|}\frac{e^2}{2h}\vec{E}. \tag{2.5}$$

It can be shown, that similarly to above, a magnetization induces a topological contribution to the charge polarization. We therefore find for the constituent equations, describing the complete electromagnetic response of the system

Constitutive Relations of Topological Insulators

$$\vec{D} = \epsilon_r\epsilon_0\vec{E} - \epsilon_0\alpha\frac{\theta}{\pi}(c_0\vec{B}) \tag{2.6}$$

$$c_0\vec{H} = \frac{c_0\vec{B}}{\mu_0\mu_r} + \alpha\frac{\theta}{\pi}\frac{\vec{E}}{\mu_0\mu_r} \tag{2.7}$$

where $\vec{D}$ describes the electric displacement field, $\vec{E}$ the electric field, $\vec{B}$ the magnetic induction and $\vec{H}$ the magnetic filed. α is the fine-structure constant and the parameter θ is quantized and takes odd integer multiples of π for topological non-trivial materials and zero otherwise. ϵ_r is the relative permittivity, ϵ_0 the permittivity of free space, μ_r the relative permeability, μ_0 the permeability of free space and c_0 the vacuum speed of light. [23]

2.3. Surface Plasmon Polaritons at Interfaces

Surface plasmons are (bosonic) electromagnetic excitations, evanescently confined in the perpendicular direction, that propagate at the interface between two media. Their appearance is most common between a dielectric and a conductor, what will become apparent when discussing the plasmon-conditions derived in this chapter. As will be shown in chapter 3 respectively in the discussion of its results following in chapter 4, under certain conditions (e.g. one of the materials being a topological insulator), a similar but more complex surface plasmon condition can also be met even if neither of the materials is a (bulk-) conductor.

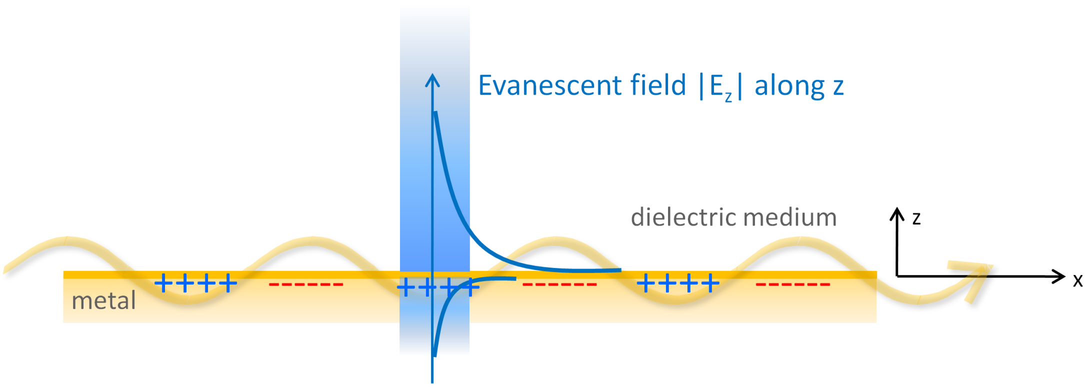

Figure 2.5.: Surface plasmons are electromagnetic waves that propagate at the interface between two media and decay exponentially in the perpendicular direction. [10]

We consider an interface between two media and look for a solution to Maxwell's equations that is exponentially damped away form the interface and propagates in the x-direction with the interface at $z = 0$. This can be done without loss of generality.

We can construct two different modes of surface plasmons: transverse magnetic (TM) and transverse electric (TE) modes, even though typically only transverse magnetic (TM) modes are realized as will be explained later.

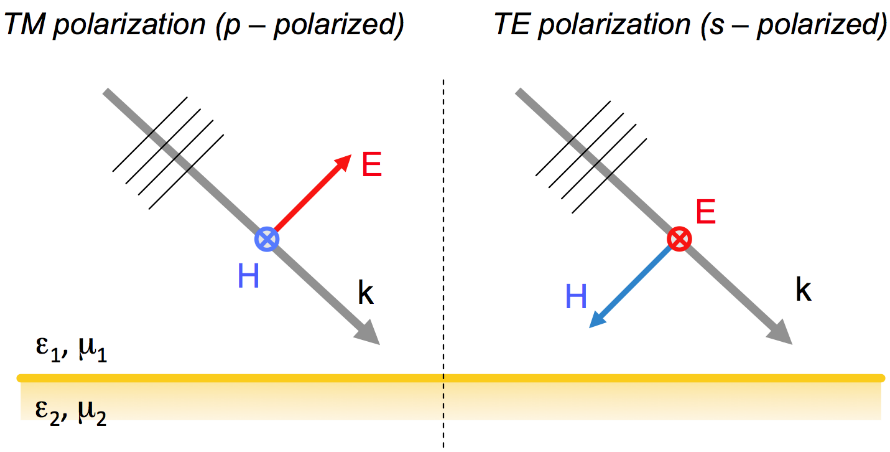

Figure 2.6.: Transverse magnetic (TM) and transverse electric (TE) modes of surface plasmons. Typically only transverse magnetic modes are realized. [10]

Let us start with transverse magnetic (TM) modes - thus we look for a solution of the form

$$\vec{H}_i = H_0 \hat{e}_y e^{i(k_x x - \omega t)} e^{i k_i^z z}, \tag{2.8}$$

where $\vec{H}$ is the magnetic field, H_0 its amplitude, $\hat{e}_y$ the unit vector in y-direction, $\vec{k}$ the wave vector, ω the frequency and x, z, t are space and time coordinates. The index i is used to distinguish between the quantities in the two different media - the regions are labeled $i = 1, 2$ for $z < 0, z > 0$.

For the plasmon to be confined in the perpendicular direction we need k_i^z to be purely imaginary with positive (negative) imaginary part for $z > 0$ ($z < 0$). This ansatz yields the following solution for Maxwell's equations

Standard Dispersion Relation

$$k_x^2 + (k_i^z)^2 = \frac{\omega^2}{c_i^2} = \epsilon_0 \epsilon_{ri} \mu_0 \mu_{ri} \omega^2, \tag{2.9}$$

which is the standard dispersion relation. ϵ_r is the relative permittivity, ϵ_0 the permittivity of free space, μ_r the relative permeability, μ_0 the permeability of free space and c_i the speed of light in medium i.

For a complete solution we also have to include the boundary conditions at an interface, which are give by

Boundary Conditions Normal Components

$$(D_{\perp 2} - D_{\perp 1}) = \sigma \tag{2.10a}$$

$$(B_{\perp 2} - B_{\perp 1}) = 0 \tag{2.10b}$$

with $\vec{D}$ the electric displacement field, $\vec{B}$ the magnetic induction and σ the surface charge density and

Boundary Conditions Parallel Components

$$\left(\vec{E}_{\parallel 2} - \vec{E}_{\parallel 1}\right) = 0 \tag{2.11a}$$

$$\left(\vec{H}_{\parallel 2} - \vec{H}_{\parallel 1}\right) = \vec{\jmath} \tag{2.11b}$$

where $\vec{E}$ is the electric field, $\vec{H}$ the magnetic field and $\vec{\jmath}$ is the surface current density.

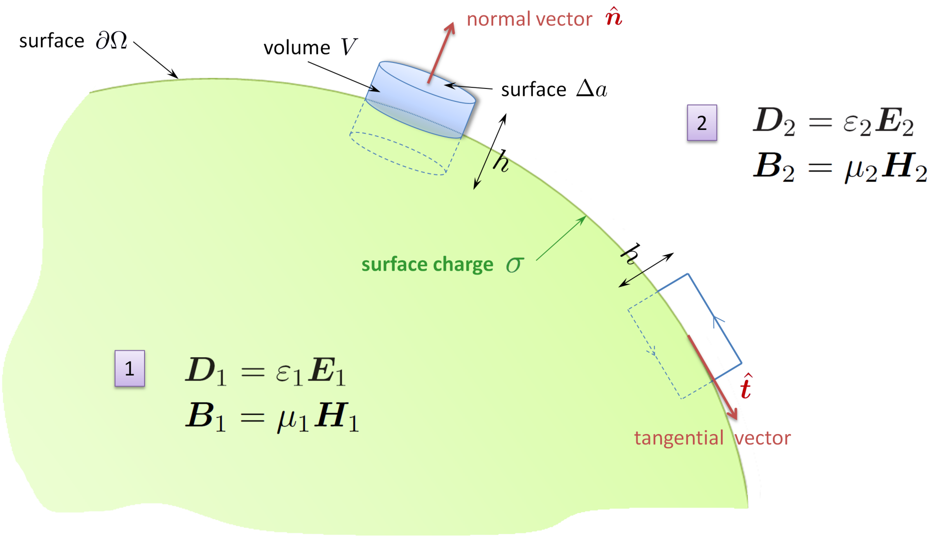

Figure 2.7.: Sketch of an interface between two different media. Using Gauss's Law (2.1a) and its magnetic analogon (2.1b) in their integral form and applying them to the volume of the small cylinder with volume V, we find in the limit of infinitesimal height ($h \rightarrow 0$) the boundary conditions for the normal components (2.10a) and (2.10b). In a similar fashion we get, applying Stoke's theorem and (2.1c) and (2.1d) to the rectangle, the boundary conditions for the tangential components (2.11a) and (2.11b) [15]

As there are no surface charges or currents in this simple case, we demand continuity of the normal component of the dielectric displacement field $\vec{D}$ as well as continuity of the parallel component of the magnetic field $\vec{H}$.

We use the standard constitutive relations in electrodynamics

Constitutive Relations

$$\vec{D} = \epsilon_0 \epsilon_r \vec{E} \tag{2.12a}$$

$$\vec{H} = \frac{\vec{B}}{\mu_0 \mu_r} \tag{2.12b}$$

and find, using Maxwell's equations

$$\vec{E} = \hat{k} \times \left(c_i \vec{B}\right), \qquad \vec{D} = -\hat{k} \times \frac{\vec{H}}{c_i} \tag{2.13}$$

and with $\hat{k} = \frac{c\vec{k}}{\omega}$, where c is the vacuum speed of light

$$\vec{D}_i = \frac{(k_i^z H_0)\hat{e}_x - (k_x H_0)\hat{e}_z}{\omega} e^{i(k_x x - \omega t)} e^{ik_i^z z} \tag{2.14}$$

As can be seen, the continuity of $\vec{H}_\parallel$ was built into our ansatz and the transverse magnetic mode $\vec{B}_\perp$ vanishes. The coefficient of $\hat{e}_z$ is independent of the index i, the medium, and therefore continuity of $\vec{D}_\parallel$ is also fulfilled. Finally, continuity of $\vec{E}_\parallel$ demands

First Plasmon Condition

$$\frac{k_2^z}{\epsilon_2} = \frac{k_1^z}{\epsilon_1}. \tag{2.15}$$

To be in accordance with our ansatz, we need opposite signs for k_i^z for the plasmon to be confined in the perpendicular direction. Assuming real ϵ_i, we find the first plasmon condition, namely the need of one of the ϵ_i to be negative.
As will be shown later, we even need a slightly stronger, additional condition to get the desired solution of a propagating plasmon:

Second Plasmon Condition

$$\epsilon_2 + \epsilon_1 < 0. \tag{2.16}$$

Now let us briefly analyze the transverse electric polarization. We look for a solution of the form

$$\vec{E}_i = E_0 \hat{e}_y e^{i(k_x x - \omega t)} e^{ik_i^z z}, \tag{2.17}$$

where $\vec{E}$ is the electric field and E_0 its amplitude, and proceed in parallel to above. In order for such a mode to exist, one finds that the permeability μ has to be negative on one side of the interface. As this condition is much harder to fulfill in practice (even though it can be met for certain frequencies in meta-materials), we assume all μ real and positive in the following and therefore no transverse electric modes to exist.

Using the standard dispersion relation (2.9) together with our first plasmon condition (2.15), we find for a surface plasmon:

Plasmon Dispersion Relation

$$k_x = \omega\sqrt{\frac{\epsilon_2\epsilon_1(\epsilon_2\mu_1 - \epsilon_1\mu_2)}{(\epsilon_2+\epsilon_1)(\epsilon_2-\epsilon_1)}} \approx \omega\sqrt{\mu\frac{\epsilon_1\epsilon_1}{\epsilon_2+\epsilon_1}}, \tag{2.18}$$

where we made the assumption $\mu_1 \approx \mu_2 = \mu$. For equal μ we further find:

$$k_i^z = i\omega\sqrt{\frac{-\mu\epsilon_i^2}{\epsilon_2+\epsilon_1}}. \tag{2.19}$$

As mentioned before, in order to find a propagating surface plasmon, there are two conditions to be satisfied for real ϵ_i. On the one hand, ϵ_i must have opposite signs on the two sides of the interface:

$$\epsilon_1\epsilon_2 < 0. \tag{2.20}$$

On the other hand, the negative ϵ_i must have a larger magnitude than the positive one:

$$\epsilon_1 + \epsilon_2 < 0. \tag{2.21}$$

Let us conclude this chapter about basic properties of surface plasmons at an interface with a popular example, namely the plasmons occurring on an interface between vacuum ($\epsilon_2 = \epsilon_0, \mu_2 = \mu_0$) and a simple Drude metal ($\mu_1 = \mu_0$) and ϵ_1 being given by the Drude relation

Drude Relation

$$\frac{\epsilon(\omega)}{\epsilon_0} = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}, \tag{2.22}$$

with the damping $\gamma = 0$ and the plasma frequency $\omega_p^2 = \frac{n_e e^2}{m\epsilon_0}$, with n_e the electron number density and m their effective mass. For the surface plasmon dispersion relation we find:

Surface Plasmon Relation Drude Model

$$k_x(\omega) = \frac{\omega}{c}\sqrt{\frac{\omega^2 - \omega_p^2}{2\omega^2 - \omega_p^2}}, \tag{2.23a}$$

$$\omega^2(k_x) = \frac{\omega_p^2}{2} + c^2 k_x^2 - \sqrt{\frac{\omega_p^4}{4} + c^4 k_x^4}. \tag{2.23b}$$

As can be seen in figure 2.8, we get a propagating surface plasmon as solution, in the range $0 < \omega < \frac{\omega_p}{\sqrt{2}}$.

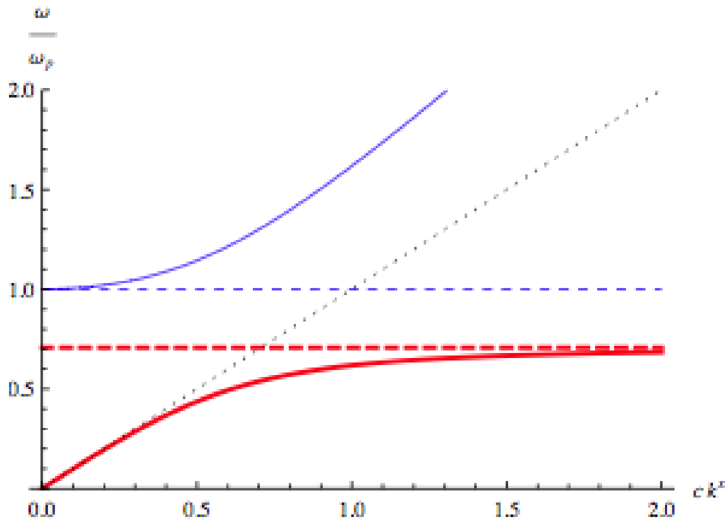

Figure 2.8.: Dispersion relation for plasmons between an ideal Drude metal ($\gamma = 0$) and vacuum. The red solid line describes the surface plasmons and the blue solid line the bulk plasmons. The black dotted line shows the dispersion relation for light $\omega = ck_x$, the blue dotted line indicates $\omega = \omega_p$ and the red dotted line $\omega = \frac{\omega_p}{\sqrt{2}}$. [19]

There exists also a second propagating solution for $\omega > \omega_p$, which is simply a propagating bulk wave in the Drude metal. As follows from (2.22), for $\omega > \omega_p$, a Drude metal has a positive ϵ. In the window $\frac{\omega_p}{\sqrt{2}} < \omega < \omega_p$ there are no propagating solutions. [19]

2.4. Dielectric Function

The dielectric function describes the response of materials to external fields. We first discuss the optical response in the independent particle approximation and start with the single particle Liouville-von-Neumann equation

Single Particle Liouville-von-Neumann Equation

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}] \tag{2.24}$$

with $\hat{\rho}$ the density operator of the system and the Hamiltonian $\hat{H}$. The Hamiltonian operator can be written as a sum of a time-independent part $\hat{H}_0$, which describes the unperturbed system, and the self-consistent potential $V(\vec{r}, t)$:

$$\hat{H} = \hat{H}_0 + V(\vec{r}, t) \tag{2.25}$$

Here, $V(\vec{r}, t)$ is the self-consistent potential consisting of the externally applied potential V_{ext} and the screening potential V_s due to the response of the electrons to the external perturbation

$$V(\vec{r}, t) = V_{ext}(\vec{r}, t) + V_s(\vec{r}, t) \tag{2.26}$$

We assume the response V_s to be classical electro-static and do not regard exchange and correlation effects here.
The motion of the electrons in the unperturbed case is described by an effective single-particle potential, which we write in the form

Eigenvalue Equation

$$\hat{H}_0|n, \vec{k}\rangle = \epsilon_{n\vec{k}}|n, \vec{k}\rangle, \tag{2.27}$$

with $|n, \vec{k}\rangle$ the Bloch state of band number n and wave vector k and $\epsilon_{n\vec{k}}$ the single-particle energy.
Applying the density operator of the unperturbed system $\hat{\rho}_0$ to the eigenstates $|n, \vec{k}\rangle$ yields

Density Operator

$$\hat{\rho}_0|n, \vec{k}\rangle = f_0(\epsilon_{n\vec{k}})|n, \vec{k}\rangle \tag{2.28}$$

where f_0 is the Fermi-Dirac distribution function.
We further assume that the density operator of the perturbed system can be decomposed into

$$\hat{\rho} = \hat{\rho}_0 + \hat{\rho}_1, \tag{2.29}$$

where $\hat{\rho}_1$ denotes the density change due the perturbation.
We can now insert (2.25), (2.26) and (2.29) into the single particle Liouville-von-Neumann equation (2.24) and obtain, by neglecting the term $[V, \hat{\rho}_1]$, the linearized form of the Liouville equation for the density change $\hat{\rho}_1$:

Linearized Single Particle Liouville-von-Neumann Equation

$$i\hbar\frac{\partial\hat{\rho}_1}{\partial t} = [\hat{H}_0, \hat{\rho}_1] + [V, \hat{\rho}_0]. \tag{2.30}$$

Furthermore, the time dependence of the external potential V_{ext} shall be given by

$$V_{ext} \sim e^{-i\omega' t}e^{\delta t} = e^{-i\omega t}, \tag{2.31}$$

with δ an infinitesimal positive number resulting in an adiabatic switching on of the perturbation. From now on the appropriate infinitesimal δ is incorporated in ω. All quantities in the linear response regime exhibit the same time dependence as the external perturbation.

We now take the matrix elements of (2.30) between the Bloch states $\langle l, \vec{k}|$ and $|m, \vec{k}+\vec{q}\rangle$. Taking into account the relations (2.27) and (2.28) this leads with a time dependence of the form $e^{-i\omega t}$ to

$$\langle l, \vec{k}|\hat{\rho}_1|m, \vec{k}+\vec{q}\rangle = \frac{f_0(\epsilon_{m\vec{k}+\vec{q}}) - f_0(\epsilon_{l\vec{k}})}{\epsilon_{m\vec{k}+\vec{q}} - \epsilon_{l\vec{k}} - \hbar\omega}\langle l, \vec{k}|V|m, \vec{k}+\vec{q}\rangle. \tag{2.32}$$

Equation (2.32) relates the induced density $\hat{\rho}_1$ to the selfconsistent potential V and will lead us to the polarizability of the system.

We use the random phase approximation (RPA), which assumes that electrons respond only to the total electric field, that is the sum of the external perturbation V_{ext} and the screening potential V_s it induces. We thus neglect the effects of local fields that vary on an atomic scale and assume the macroscopic external perturbation to produce a screening potential only on a macroscopic scale. Therefore, the total perturbation potential V, being the sum of the externally applied potential V_{ext} and the screening potential V_s, can be expressed as a Fourier series of the form

Fourier Series of Total Perturbation Potential

$$V(\vec{r}, t) = \sum_{\vec{q}} V(\vec{q}, t)e^{-i\vec{q}\cdot\vec{r}}. \tag{2.33}$$

Inserting this expression into the right hand side of (2.34) gives

$$\langle l, \vec{k}|\hat{\rho}_1|m, \vec{k}+\vec{q}\rangle = \frac{f_0(\epsilon_{m\vec{k}+\vec{q}}) - f_0(\epsilon_{l\vec{k}})}{\epsilon_{m\vec{k}+\vec{q}} - \epsilon_{l\vec{k}} - \hbar\omega}V(\vec{q}, t)\langle l, \vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m, \vec{k}+\vec{q}\rangle, \tag{2.34}$$

where the sum over $\vec{q}$ has dropped out due to conservation of crystal momentum.

We use the following relation to find the induced charge density $n(\vec{r})$:

Induced Charge Density

$$\begin{aligned} n(\vec{r}) &= \mathrm{Tr}[\delta(\vec{r}-\vec{r}_e)\hat{\vec{\rho}}_1] \\ &= \sum_{\vec{q}} \sum_{lm\vec{k}} \psi^{\dagger}_{m\vec{k}+\vec{q}}(\vec{r})\psi_{l\vec{k}}(\vec{r})\langle l,\vec{k}|\hat{\rho}_1|m,\vec{k}+\vec{q}\rangle, \end{aligned} \tag{2.35}$$

which reads in the reciprocal space

$$n(\vec{q}) = \sum_{lm\vec{k}} \langle l,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m,\vec{k}+\vec{q}\rangle^{\dagger}\langle l,\vec{k}|\hat{\rho}_1|m,\vec{k}+\vec{q}\rangle. \tag{2.36}$$

Inserting (2.34) into the right hand side of (2.36) yields

$$n(\vec{q},\omega) = \sum_{lm\vec{k}} \frac{f_0(\epsilon_{m\vec{k}+\vec{q}}) - f_0(\epsilon_{l\vec{k}})}{\epsilon_{m\vec{k}+\vec{q}} - \epsilon_{l\vec{k}} - \hbar\omega} \langle l,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m,\vec{k}+\vec{q}\rangle^{\dagger}\langle l,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m,\vec{k}+\vec{q}\rangle V(\vec{q},\omega), \tag{2.37}$$

which relates the induced charge density n with the total perturbing potential V. By comparison of (2.37) with the definition of the polarization $\hat{P}^0$ via the relation between induced charge ρ_{ind} and perturbing potential

Relation between ρ_{ind} and $\hat{P}^0(\vec{q},\omega)$

$$\rho_{ind} = n(\vec{q},\omega)\Omega = \hat{P}^0(\vec{q},\omega)V(\vec{q},\omega), \tag{2.38}$$

where Ω is the crystal volume, we can easily identify the polarization as:

Polarization Function

$$\hat{P}^0(\vec{q},\omega) = \frac{1}{\Omega}\sum_{lm\vec{k}} \frac{f_0(\epsilon_{m\vec{k}+\vec{q}}) - f_0(\epsilon_{l\vec{k}})}{\epsilon_{m\vec{k}+\vec{q}} - \epsilon_{l\vec{k}} - \hbar\omega} \langle l,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m,\vec{k}+\vec{q}\rangle^\dagger \langle l,\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m,\vec{k}+\vec{q}\rangle. \tag{2.39}$$

Using Poissons's equation and the definition of the dielectric function ϵ as the relation between the external potential V_{ext} and the total potential V,

$$V_{ext} = \epsilon V, \tag{2.40}$$

we find the following expression for the macroscopic dielectric function:

Macroscopic Dielectric Function

$$\epsilon(\vec{q},\omega) = 1 - \nu(\vec{q})\hat{P}^0(\vec{q},\omega), \tag{2.41}$$

with the Fourier transform of the Coulomb potential $\nu(\vec{q})$. [30]

3. Modeling

Like in the previous chapter we look for a wave solution to Maxwells'equations that propagates along an interface between two dielectrics. With the interface at $z = 0$, we can take the x-direction to be the direction of propagation, without loss of generality. To model the bulk behavior of the topological insulator we take one dielectric to have a relative permittivity in the typical range of an insulator. In case of the topological insulator Bismuth telluride (Bi_2Te_3) $\epsilon_r \approx 50$ [1]. In order to implement the effects occurring on the surface of the topological insulator, we use new constitutive relations in electromagnetism and add surface charges (originating form free massless Dirac electrons) and surface currents to our system.

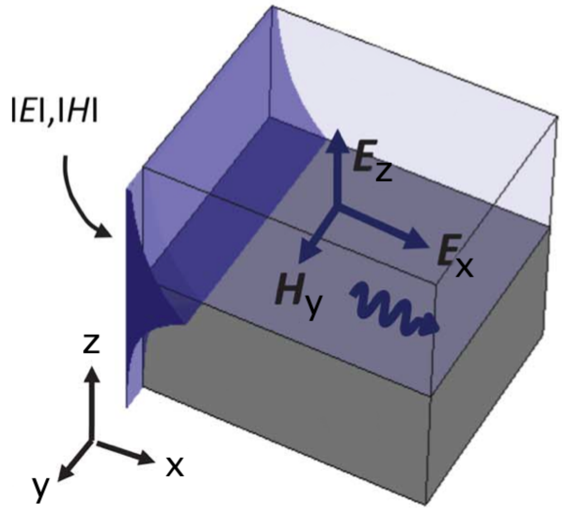

Figure 3.1.: We model plasmons in topological insulators with a two layer system (describing the bulk of the topological insulator on the one side and a normal dielectric on the other side of the interface) with surface charges and surface currents originating from free massless Dirac electrons. Without loss of generality, we take the x-direction to be the direction of propagation and demand exponential decay of the electric and magnetic fields in order to find a localized mode. [14]

In section 3.1 we use these new constitutive relations describing a topological insulator and a general ansatz for the surface plasmons, that incorporates transversal electric (TE) and transversal magnetic (TM) modes, to calculate the boundary conditions on our interface and to find a general expression for the plasmon condition.

The optical conductivity in two dimensions is derived in section 3.2 and is needed to make a connection between the surface charges and currents found on the surface of a topological insulator and the electronic properties of a two dimensional free massless Dirac electron gas.

In the last section of chapter 3 we calculate for a 2D gas consisting of free massless Dirac electrons the dynamical polarization within the random phase approximation (RPA) for arbitrary wave vector, frequency and doping.

3.1. Surface Plasmon Condition

Using new constitutive relations in electromagnetism, we will derive general expressions for the electric displacement field $\vec{D}$ and the magnetic field $\vec{H}$ on an interface in section 3.1.1. With the standard boundary conditions of electrodynamics we will find the general expression for the plasmon condition incorporating topological effects in section 3.1.2.

3.1.1. Constitutive Relations of Topological Insulators

In SI units the constitutive relations describing a topological insulator (TI) read

Constitutive Relations of Topological Insulators

$$\vec{D} = \epsilon_r \epsilon_0 \vec{E} - \epsilon_0 \alpha \frac{\theta}{\pi}(c_0 \vec{B}) \tag{3.1}$$

$$c_0 \vec{H} = \frac{c_0 \vec{B}}{\mu_0 \mu_r} + \alpha \frac{\theta}{\pi} \frac{\vec{E}}{\mu_0 \mu_r} \tag{3.2}$$

where $\vec{D}$ describes the electric displacement field, $\vec{E}$ the electric field, $\vec{B}$ the magnetic induction and $\vec{H}$ the magnetic filed. α is the fine-structure constant and the parameter θ is quantized and takes odd integer multiples of π for topological non-trivial materials and zero otherwise. ϵ_r is the relative permittivity, ϵ_0 the permittivity of free space, μ_r the relative permeability, μ_0 the permeability of free space and c_0 the vacuum speed of light with

Speed of Light in Vacuum

$$c_0 = \frac{1}{\sqrt{\mu_0 \epsilon_0}}. \tag{3.3}$$

The speed of light in medium r is connected with the materials permittivity and permeability via the following relation:

Speed of Light in Medium

$$c_r = \frac{1}{\sqrt{\mu_0 \mu_r \epsilon_0 \epsilon_r}}, \tag{3.4}$$

Maxwell's equations themselves are not modified. The consideration of the topological magneto-electric effect (TME) in form of modified constitutive relations is only valid when the massless topological surface modes are gapped.

We use a general wave ansatz for $\vec{E}$, which allows for TE (transversal electric) and TM (transversal magnetic) modes:

Ansatz for $\vec{E}$ component of Plasmon Mode

$$\vec{E}_i = \left[E_{TE}\hat{e}_y + \frac{c_i E^i_{TM}}{\omega}\left(k_x \hat{e}_z - k^z_i \hat{e}_x\right)\right] e^{\imath(k_x - \omega t)} e^{\imath k^z_i z} \tag{3.5}$$

The index i is used to distinguish between the quantities in the two different media. E_{TE} is the amplitude of the TE mode, E_{TM} the amplitude of the TM mode and $\hat{e}_x, \hat{e}_y, \hat{e}_z$ are the unit vectors that span our basis system. c, ω, k stand for the speed of light, the frequency and the wave vector respectively, and t stands for time. We are interested in a plasmon like solution where k^z_i is purely imaginary, with opposite signs on the two sides of the interface.

As we stated in chapter 2.3 about surface plasmon polaritons at interfaces, we have to include boundary conditions at the boundary surface in order to find a complete solution. For the parallel component of the electric field $\vec{E}$ we found its components to be continuous across the border (2.7a). Given the geometry of our model, with the interface at z=0 and the x-direction the direction of propagation, we demand continuity of E_y and E_x. Continuity of E_y is already incorporated in our ansatz, continuity of E_x leads to the non-trivial conditions on the TM mode:

$$E_1^x \propto \frac{c_1 E_{TM}^1}{\omega}\left(-k_1^z\right) \quad \wedge \quad E_2^x \propto \frac{c_2 E_{TM}^2}{\omega}\left(-k_2^z\right) \tag{3.6}$$

which leads to

$$\Rightarrow c_1 E_{TM}^1 k_1^z = c_2 E_{TM}^2 k_2^z \tag{3.7}$$

For a plane wave solution we have the standard dispersion relation

Standard Dispersion Relation

$$k_x^2 + (k_i^z)^2 = \frac{\omega^2}{c_i^2} = \epsilon_0 \epsilon_{ri} \mu_0 \mu_{ri} \omega^2 \tag{3.8}$$

Furthermore, we obtain from Maxwell's equations relations between $\vec{E}$ and $\vec{B}$ respectively $\vec{D}$ and $\vec{H}$:

$$\vec{E} = -\hat{k} \times \left(c_i \vec{B}\right) \tag{3.9}$$

$$\vec{D} = -\hat{k} \times \frac{\vec{H}}{c_i} \tag{3.10}$$

with the abbreviation $\hat{k}$ for the normalized wave vector

$$\hat{k} = \frac{c\vec{k}}{\omega}. \tag{3.11}$$

This leads with

$$\vec{B} = \frac{1}{c}\hat{k} \times \vec{E} \tag{3.12}$$

to

$$\frac{c_i E^i_{TM}}{\omega}\begin{pmatrix} k_x \\ 0 \\ k^z_i \end{pmatrix} \times \begin{pmatrix} k^z_i \\ 0 \\ k_x \end{pmatrix} = \frac{c_i E^i_{TM}}{\omega}\begin{pmatrix} 0 \\ -\left(k_x^2 + (k^z_i)^2\right) \\ 0 \end{pmatrix} = -\frac{E^i_{TM}}{c_i}\hat{e}_y \tag{3.13}$$

for the TM mode, and to

$$\frac{c\vec{k}}{\omega} \times E_{TE}\hat{e}_y = \frac{1}{\omega}\begin{pmatrix} k_x \\ k_y \\ k^z_i \end{pmatrix} \times \begin{pmatrix} 0 \\ E_{TE} \\ 0 \end{pmatrix} = \frac{1}{\omega}\left(-k^z_i E_{TE}\hat{e}_x + k_x E_{TE}\hat{e}_z\right) \tag{3.14}$$

for the TE mode.
We therefore find for the magnetic induction $\vec{B}$:

$\vec{B}$ component of Plasmon Mode

$$\vec{B}_i = \left[\frac{(k_x E_{TE})\,\hat{e}_z - (k^z_i E_{TE})\,\hat{e}_x}{\omega} - \frac{E^i_{TM}}{c_i}\hat{e}_y\right] e^{\imath(k_x - \omega t)} e^{\imath k^z_i z} \tag{3.15}$$

From the boundary condition (2.6b) for the normal component of the magnetic induction $\vec{B}$, we demand continuity of $B_\perp = B_z$ in our model, which is automatically satisfied, as the coefficient of $\hat{e}_z$ is identical on both sides of the interface.

Having expressed the the magnetic induction $\vec{B}$ component of the plasmon mode in terms of components of the electric field $\vec{E}$, we can now simply insert (3.5) and (3.15) in the constitutive relations of topological insulators (3.1) and (3.2) and find for $\vec{D}$ and $\vec{H}$ the following expressions [19]:

$\vec{D}$ and $\vec{H}$ from Constitutive Relations

$$\vec{D}_i = \Bigg\{ \epsilon_0 \epsilon_{ri} \left[E_{TE} \hat{e}_y + \frac{c_i E^i_{TM}}{\omega} \left(k_x \hat{e}_z - k^z_i \hat{e}_x \right) \right] - \epsilon_0 \alpha \frac{\theta}{\pi} c_0 \left[\frac{\left(k_x E_{TE} \right) \hat{e}_z - \left(k^z_i E_{TE} \right) \hat{e}_x}{\omega} - \frac{E^i_{TM}}{c_i} \hat{e}_y \right] \Bigg\} e^{\imath (k_x - \omega t)} e^{\imath k^z_i z} \tag{3.16}$$

$$c_0 \vec{H}_i = \Bigg\{ \frac{c_0}{\mu_0 \mu_i} \left[\frac{\left(k_x E_{TE} \right) \hat{e}_z - \left(k^z_i E_{TE} \right) \hat{e}_x}{\omega} - \frac{E^i_{TM}}{c_i} \hat{e}_y \right] + \alpha \frac{\theta}{\pi} \frac{\left[E_{TE} \hat{e}_y + \frac{c_i E^i_{TM}}{\omega} \left(k_x \hat{e}_z - k^z_i \hat{e}_x \right) \right]}{\mu_0 \mu_r} \Bigg\} e^{\imath (k_x - \omega t)} e^{\imath k^z_i z} \tag{3.17}$$

3.1.2. Boundary Conditions

The boundary conditions of an interface with surface charges and surface currents (not the Hall-current which is taken into account by the modified constitutive relations) are:

Boundary Conditions for $D_\perp$ and $B_\perp$

$$\left(D_{\perp 2} - D_{\perp 1} \right) = \sigma \tag{3.18a}$$

$$\left(B_{\perp 2} - B_{\perp 1} \right) = 0 \tag{3.18b}$$

with σ the surface charge density, and

Boundary Conditions for $\vec{E}_\parallel$ and $\vec{H}_\parallel$

$$\left(\vec{E}_{\parallel 2} - \vec{E}_{\parallel 1}\right) = 0 \tag{3.19a}$$

$$\left(\vec{H}_{\parallel 2} - \vec{H}_{\parallel 1}\right) = \vec{\jmath} \tag{3.19b}$$

where $\vec{\jmath}$ is the surface current density. [15] In the previous chapter 3.1.1 we already used the fact, that the parallel component of the electric field $\vec{E}$ and the normal component of the magnetic induction $\vec{B}$ are continuous across the interface, to derive the electric displacement component and the magnetic field component of a plasmon in terms of the electric field. We now use the two remaining conditions to find relations between the amplitudes of the TE and TM modes of the plasmon (similar to [19]).

From $(D_{\perp 2} - D_{\perp 1}) = \sigma$ we find

$$\epsilon_0 \epsilon_{r2} \frac{c_2 E^2_{TM}}{\omega} k_x - \epsilon_0 \alpha \frac{\theta_2}{\pi} c_0 \frac{k_x E_{TE}}{\omega} - \left(\epsilon_0 \epsilon_{r1} \frac{c_1 E^1_{TM}}{\omega} k_x - \epsilon_0 \alpha \frac{\theta_1}{\pi} c_0 \frac{k_x E_{TE}}{\omega} \right) = \sigma, \tag{3.20}$$

which, using $c_1 E^1_{TM} k^z_1 = c_2 E^2_{TM} k^z_2$ and $\Delta\theta = \theta_1 - \theta_2$, can be further simplified to

$$\epsilon_0 \epsilon_{r2} \frac{c_2 E^1_{TM}}{\omega} \frac{k^z_1}{k^z_2} k_x - \left(\epsilon_0 \epsilon_{r1} \frac{c_1 E^1_{TM}}{\omega} k_x + \epsilon_0 \alpha \frac{\Delta\theta}{\pi} c_0 \frac{k_x E_{TE}}{\omega} \right) = \sigma \tag{3.21}$$

$$\epsilon_0 c_1 E^1_{TM} \left(\epsilon_{r2} \frac{k^z_1}{k^z_2} - \epsilon_{r1} \right) + \epsilon_0 c_0 E_{TE} \alpha \frac{\Delta\theta}{\pi} = \frac{\sigma\omega}{k_x}. \tag{3.22}$$

This relates the TE to the TM amplitude according to

Relation between TE and TM Amplitude from Condition for $\boldsymbol{D}_\perp$

$$E^1_{TM} = \frac{\alpha\left(\frac{\Delta\theta}{\pi}\right)\epsilon_0 c_0}{c_1\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k^z_1}{k^z_2}\right)} E_{TE} - \frac{\sigma\omega}{k_x c_1 \epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k^z_1}{k^z_2}\right)}. \tag{3.23}$$

$\left(\vec{H}_{\|2} - \vec{H}_{\|1}\right) = \vec{\jmath}$ leads to two conditions, one for the x-component of the magnetic field and one for its y-component. For the for the x-component we find the condition:

$$k^z_2\left(\frac{E_{TE}}{\mu_0\mu_{r2}} + \alpha\frac{\theta_2}{\pi}\frac{c_2}{c_0\mu_0}E^2_{TM}\right) - k^z_1\left(\frac{E_{TE}}{\mu_0\mu_{r1}} + \alpha\frac{\theta_1}{\pi}\frac{c_1}{c_0\mu_0}E^1_{TM}\right) = j_y. \tag{3.24}$$

Remembering that $c_1 E^1_{TM} k^z_1 = c_2 E^2_{TM} k^z_2$ and $\Delta\theta = \theta_1 - \theta_2$, this expression can be further simplified:

$$k^z_2\frac{E_{TE}}{\mu_0\mu_{r2}} + \alpha\frac{\theta_2}{\pi}\frac{1}{c_0\mu_0}k^z_2 c_2 E^1_{TM} - k^z_1\frac{E_{TE}}{\mu_0\mu_{r1}} + \alpha\frac{\theta_1}{\pi}\frac{1}{c_0\mu_0}k^z_1 c_1 E^1_{TM} = j_y \tag{3.25}$$

$$E^1_{TM}\alpha\frac{\Delta\theta}{\pi}\frac{c_1 k^z_1}{c_0\mu_0} - E_{TE}\left(\frac{k^z_2}{\mu_0\mu_{r2}} - \frac{k^z_1}{\mu_0\mu_{r1}}\right) - j_y \tag{3.26}$$

and we arrive at

1st Relation between TE and TM Amplitude from Condition for $\vec{\boldsymbol{H}}_\|$

$$E^1_{TM} = \frac{\mu_{r1}\left(\frac{k^z_2}{k^z_1}\right) - \mu_{r2}}{\alpha\frac{\Delta\theta}{\pi}\mu_{r1}\mu_{r2}c_1}\mu_0 c_0 E_{TE} - \frac{c_0\mu_0}{\alpha\frac{\Delta\theta}{\pi}c_1 k^z_1}j_y \tag{3.27}$$

Likewise, $\left(\vec{H}_{\|2} - \vec{H}_{\|1}\right) = \vec{\jmath}$ leads to the following condition for the y-component:

$$-\frac{E^2_{TM}}{c_2\mu_0\mu_{r2}} + \alpha\frac{\theta_2}{\pi}\frac{E_{TE}}{\mu_0 c_0} - \left(-\frac{E^1_{TM}}{c_1\mu_0\mu_{r1}} + \alpha\frac{\theta_1}{\pi}\frac{E_{TE}}{\mu_0 c_0}\right) = -j_x \tag{3.28}$$

$$-\frac{c_1 E_{TM}^1 k_1^z}{c_2^2 \mu_0 \mu_{r2} k_2^z} + \alpha \frac{\theta_2}{\pi} \frac{E_{TE}}{\mu_0 c_0} + \frac{E_{TM}^1}{c_1 \mu_0 \mu_{r1}} - \alpha \frac{\theta_1}{\pi} \frac{E_{TE}}{\mu_0 c_0} = -j_x \tag{3.29}$$

$$c_1 E_{TM}^1 \left(\frac{1}{c_1^2 \mu_0 \mu_{r1}} - \frac{1}{c_2^2 \mu_0 \mu_{r2}} \frac{k_1^z}{k_2^z} \right) = \alpha \frac{\Delta\theta}{\pi} \frac{E_{TE}}{\mu_0 c_0} - j_x, \tag{3.30}$$

which, using $c_0 = \frac{1}{\sqrt{\mu_0 \epsilon_0}}$, can be further reduced to

$$c_1 E_{TM}^1 \left(\epsilon_0 \epsilon_{r1} - \epsilon_0 \epsilon_{r2} \frac{k_1^z}{k_2^z} \right) = \alpha \frac{\Delta\theta}{\pi} \frac{E_{TE} \epsilon_0}{\epsilon_0 \mu_0 c_0} - j_x \tag{3.31}$$

$$c_1 E_{TM}^1 \left(\epsilon_0 \epsilon_{r1} - \epsilon_0 \epsilon_{r2} \frac{k_1^z}{k_2^z} \right) = \alpha \frac{\Delta\theta}{\pi} E_{TE} \epsilon_0 c_0 - j_x \tag{3.32}$$

and yields

2nd Relation between TE and TM Amplitude from Condition for $\vec{H}_{\parallel}$

$$E_{TM}^1 = \frac{\alpha \frac{\Delta\theta}{\pi} c_0}{c_1 \left(\epsilon_{r1} - \epsilon_{r2} \frac{k_1^z}{k_2^z} \right)} E_{TE} - \frac{1}{c_1 \left(\epsilon_0 \epsilon_{r1} - \epsilon_0 \epsilon_{r2} \frac{k_1^z}{k_2^z} \right)} j_x. \tag{3.33}$$

We got three equations relating the TE to the TM amplitude of the plasmons electric field. As can be shown straight forwardly for the case without charges and currents at the boundary, by simply setting $\sigma = 0$ and $j_x = 0$ in equations (3.23) and (3.33), the two conditions are redundant. For the two conditions $(D_{\perp 2} - D_{\perp 1}) = \sigma$ and $\left(\vec{H}_{\parallel 2y} - \vec{H}_{\parallel 1y}\right) = \vec{j}$ to be redundant in the case for $\sigma \neq 0$, $\vec{j} \neq \vec{0}$ we get:

Redundancy of $(D_{\perp 2} - D_{\perp 1}) = \sigma$ and $\left(\vec{H}_{\parallel 2y} - \vec{H}_{\parallel 1y}\right) = \vec{j}$

$$\frac{\sigma\omega}{k_x c_1 \left(\epsilon_0\epsilon_{r1} - \epsilon_0\epsilon_{r2}\frac{k_1^z}{k_2^z}\right)} = \frac{j_x}{c_1 \left(\epsilon_0\epsilon_{r1} - \epsilon_0\epsilon_{r2}\frac{k_1^z}{k_2^z}\right)} \tag{3.34}$$

$$\sigma\omega = j_x k_x, \tag{3.35}$$

which is simply the continuity equation.

So we are left with the only two conditions

$$E_{TM}^1 = \frac{\mu_1\left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\alpha\frac{\Delta\theta}{\pi}\mu_1\mu_2 c_1}\mu_0 c_0 E_{TE} - \frac{c_0\mu_0}{\alpha\frac{\Delta\theta}{\pi}c_1 k_1^z}j_y\omega \tag{3.36}$$

with $\mu_i = \mu_0\mu_r$ and

$$E_{TM}^1 = \frac{\alpha\left(\frac{\Delta\theta}{\pi}\right)\epsilon_0 c_0}{c_1\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right)}E_{TE} - \frac{\sigma\omega}{k_x c_1\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right)}. \tag{3.37}$$

In the next step we will relate the charge density as well as the current density to the two dimensional conductivity $\bar{\sigma}_{2D}$, which will be connected to the dielectric function in chapter 3.2.

We start with Ohm's law

Ohm's law

$$\vec{J} = \bar{\sigma} \cdot \vec{E} \tag{3.38}$$

with $\vec{J}$ the current density and $\bar{\sigma}$ the conductivity and the continuity equation

Fouriertransform of Continuity equation

$$\rho\omega = \vec{J} \cdot \vec{k}. \tag{3.39}$$

We find for j_y in equation (3.18) and σ in equation (3.19):

Relation between Charge Density, Current Density and Conductivity

$$j_y = \bar{\sigma}_{2D} E_{TE} \tag{3.40}$$

$$\sigma = \frac{j_x k_x}{\omega} = -\frac{\bar{\sigma}_{2D} c_1 k_1^z k_x}{\omega^2} E_{TM}^1, \tag{3.41}$$

where $\bar{\sigma}_{2D}$ describes the two dimensional conductivity.

Using the expressions (3.40) and (3.41) for the charge- and current density, equations (3.18) and (3.19) become

$$E_{TM}^1 = \frac{\mu_1 \left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\alpha \frac{\Delta\theta}{\pi} \mu_1 \mu_2 c_1} \mu_0 c_0 E_{TE} - \frac{c_0 \mu_0}{\alpha \frac{\Delta\theta}{\pi} c_1 k_1^z} \bar{\sigma}_{2D} \omega E_{TE} \tag{3.42}$$

$$E_{TM}^1 = \left(\frac{\mu_1 \left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\mu_1 \mu_2} - \frac{\bar{\sigma}_{2D}\omega}{k_1^z} \right) \frac{c_0 \mu_0}{\alpha \frac{\Delta\theta}{\pi} c_1} E_{TE} \tag{3.43}$$

and

$$E_{TM}^1 = \frac{\alpha \left(\frac{\Delta\theta}{\pi}\right) \epsilon_0 c_0}{c_1 \epsilon_0 \left(\epsilon_{r1} - \epsilon_{r2} \frac{k_1^z}{k_2^z}\right)} E_{TE} + \frac{\omega}{k_x c_1 \epsilon_0 \left(\epsilon_{r1} - \epsilon_{r2} \frac{k_1^z}{k_2^z}\right)} \frac{\bar{\sigma}_{2D} c_1 k_1^z k_x}{\omega^2} E_{TM}^1 \tag{3.44}$$

$$\left(c_1 \epsilon_0 \left(\epsilon_{r1} - \epsilon_{r2} \frac{k_1^z}{k_2^z} \right) - \frac{\bar{\sigma}_{2D} c_1 k_1^z}{\omega} \right) E_{TM}^1 = \alpha \left(\frac{\Delta\theta}{\pi} \right) \epsilon_0 c_0 E_{TE} \tag{3.45}$$

$$E^{1}_{TM} = \frac{\alpha\left(\frac{\Delta\theta}{\pi}\right)\epsilon_0 c_0}{\left(c_1\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right) - \frac{\bar{\sigma}_{2D} c_1 k_1^z}{\omega}\right)} E_{TE} \tag{3.46}$$

To simultaneously satisfy the two equations, relating the TE and TM amplitudes, we need

$$\left(\frac{\mu_1\left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\mu_1\mu_2} - \frac{\bar{\sigma}_{2D}\omega}{k_1^z}\right)\frac{c_0\mu_0}{\alpha\frac{\Delta\theta}{\pi}c_1} = \frac{\alpha\left(\frac{\Delta\theta}{\pi}\right)\epsilon_0 c_0}{\left(c_1\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right) - \frac{\bar{\sigma}_{2D} c_1 k_1^z}{\omega}\right)}. \tag{3.47}$$

We hereby find the plasmon condition for topological insulators, respectively a general plasmon condition for interfaces with surface charges and surface currents of non trivial topological order.

Plasmon Condition for Topological Insulators

$$\left(\frac{\mu_1\left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\mu_1\mu_2} - \frac{\bar{\sigma}_{2D}\omega}{k_1^z}\right)\left(\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right) - \frac{\bar{\sigma}_{2D}k_1^z}{\omega}\right) = \left(\alpha\frac{\Delta\theta}{\pi}\right)^2\frac{\epsilon_0}{\mu_0} \tag{3.48}$$

For $\bar{\sigma}_{2D} = 0$ and $\Delta\theta = 0$, this yields the standard equations found previously:

Standard Plasmon Condition

$$\left(\frac{\mu_1\left(\frac{k_2^z}{k_1^z}\right) - \mu_2}{\mu_1\mu_2}\right)\left(\epsilon_0\left(\epsilon_{r1} - \epsilon_{r2}\frac{k_1^z}{k_2^z}\right)\right) = 0 \tag{3.49}$$

with the solutions

1st Solution to Standard Plasmon Condition

$$\frac{\epsilon_1}{k_1^z} = \frac{\epsilon_2}{k_2^z} \tag{3.50}$$

and

2nd Solution to Standard Plasmon Condition

$$\mu_1 k_2^z = \mu_2 k_1^z \tag{3.51}$$

where we used the abbreviations $\epsilon_i = \epsilon_0 \epsilon_r$ and $\mu_i = \mu_0 \mu_r$. As the second solution requires negative μ, this TE surface plasmon is typically not realized.

In the following we set $\mu_i = \mu_0$.
Including the effects of $\bar{\sigma}_{2D}$ and $\Delta\theta$, we get two solutions for k_1^z:

1st Solution to Plasmon Condition for TI

$$\begin{aligned} k_1^z = \frac{1}{2\pi^2 \left(\bar{\sigma}_{2D} k_2^z + \omega\epsilon_2\right)} \Big[& \alpha^2 \Delta\theta^2 \omega \epsilon_0 k_2^z - \pi^2 \mu_0 \bar{\sigma}_{2D}^2 \omega k_2^z + \\ & + \pi^2 \bar{\sigma}_{2D} (k_2^z)^2 + \pi^2 \omega \epsilon_1 k_2^z + \pi^2 \omega \epsilon_2 k_2^z - \pi^2 \mu_0 \bar{\sigma}_{2D} \omega^2 \epsilon_2 + \\ & + \left\{ \left(\omega k_2^z \left(\alpha^2 \Delta\theta^2 \epsilon_0 - \pi^2 \mu_0 \bar{\sigma}_{2D}^2 + \pi^2 \left(\epsilon_1 + \epsilon_2\right)\right) + \pi^2 \bar{\sigma}_{2D} (k_2^z)^2 - \pi^2 \mu_0 \bar{\sigma}_{2D} \omega^2 \epsilon_2 \right)^2 + \right. \\ & \left. + 4\pi^4 \omega \epsilon_1 k_2^z \left(\mu_0 \bar{\sigma}_{2D} \omega - k_2^z\right) \left(\bar{\sigma}_{2D} k_2^z + \omega \epsilon_2\right) \right\}^{\frac{1}{2}} \Big] \end{aligned} \tag{3.52}$$

and

2nd Solution to Plasmon Condition for TI

$$k_1^z = \frac{1}{2\pi^2\left(\bar{\sigma}_{2D}k_2^z + \omega\epsilon_2\right)}\Big[\alpha^2\Delta\theta^2\omega\epsilon_0 k_2^z - \pi^2\mu_0\bar{\sigma}_{2D}^2\omega k_2^z +$$
$$+\pi^2\bar{\sigma}_{2D}(k_2^z)^2 + \pi^2\omega\epsilon_1 k_2^z + \pi^2\omega\epsilon_2 k_2^z - \pi^2\mu_0\bar{\sigma}_{2D}\omega^2\epsilon_2$$
$$-\Big\{\Big(\omega k_2^z\left(\alpha^2\Delta\theta^2\epsilon_0 - \pi^2\mu_0\bar{\sigma}_{2D}^2 + \pi^2\left(\epsilon_1+\epsilon_2\right)\right) + \pi^2\bar{\sigma}_{2D}(k_2^z)^2 - \pi^2\mu_0\bar{\sigma}_{2D}\omega^2\epsilon_2\Big)^2 +$$
$$+4\pi^4\omega\epsilon_1 k_2^z\left(\mu_0\bar{\sigma}_{2D}\omega - k_2^z\right)\left(\bar{\sigma}_{2D}k_2^z + \omega\epsilon_2\right)\Big\}^{\frac{1}{2}}\Big] \tag{3.53}$$

We will use the second result, as it describes an evanescent wave in medium 1.

In order to have a localized mode we need k_2^z to be

Localized Mode Condition

$$k_2^z = -\sqrt{\frac{\omega^2}{\frac{c^2}{\frac{\epsilon_2}{\epsilon_0}}}} \tag{3.54}$$

which is obtained straight forwardly from the standard dispersion relation

$$k_x^2 + (k_i^z)^2 = \epsilon_i\mu_i\omega^2. \tag{3.55}$$

The equation describing the dispersion relation of plasmons confined at the surface between two media, with surface charges, surface currents and topological effects, is therefore given by inserting the result for k_1^z from equation (3.53) into the standard dispersion relation (3.55):

Plasmon Dispersion Relation of Topological Insulators

$$
\begin{aligned}
k_x^2 = \epsilon_i\mu_i\omega^2 - \Bigg(& \frac{1}{2\pi^2\left(\bar{\sigma}_{2D}k_2^z + \omega\epsilon_2\right)} \left[\alpha^2\Delta\theta^2\omega\epsilon_0 k_2^z - \pi^2\mu_0\bar{\sigma}_{2D}^2\omega k_2^z + \right. \\
& + \pi^2\bar{\sigma}_{2D}(k_2^z)^2 + \pi^2\omega\epsilon_1 k_2^z + \pi^2\omega\epsilon_2 k_2^z - \pi^2\mu_0\bar{\sigma}_{2D}\omega^2\epsilon_2 \\
& - \Big\{\Big(\omega k_2^z\left(\alpha^2\Delta\theta^2\epsilon_0 - \pi^2\mu_0\bar{\sigma}_{2D}^2 + \pi^2\left(\epsilon_1+\epsilon_2\right)\right) + \pi^2\bar{\sigma}_{2D}(k_2^z)^2 - \pi^2\mu_0\bar{\sigma}_{2D}\omega^2\epsilon_2\Big)^2 + \\
& \left. + 4\pi^4\omega\epsilon_1 k_2^z\left(\mu_0\bar{\sigma}_{2D}\omega - k_2^z\right)\left(\bar{\sigma}_{2D}k_2^z + \omega\epsilon_2\right)\Big\}^{\frac{1}{2}}\right]\Bigg)^2 .
\end{aligned}
\tag{3.56}
$$

3.2. Optical Conductivity in 2D

In order to evaluate the plasmon dispersion relation of topological insulators (3.56), found in chapter 3.1.2, we have to determine the 2D conductivity of a 2D free massless Dirac electron gas. We therefore derive the common relation relation between the 2D conductivity $\bar{\sigma}_{2D}$ and the 2D dielectric function in this section, before calculating the permittivity of surface states of topological insulators in the next section.

We use the Fourier transform of Ohm's law

Fourier Transform of Ohm's Law

$$\vec{J} = \bar{\sigma}\vec{E} \tag{3.57}$$

with $\vec{J}$ the current density and $\bar{\sigma}$ the conductivity and the Fourier transform of the continuity equation, which can be expressed as

Fourier Transform of Continuity Equation

$$\rho\omega = \vec{J} \cdot \vec{k}. \tag{3.58}$$

where ρ is the electric charge density. We further find for a (longitudinal) electric field

$$\vec{E} = \vec{\nabla} V \quad \Rightarrow \quad \vec{E}_l(\vec{q}, \omega) = -i\vec{q}V, \tag{3.59}$$

where V is the electric potential and $\vec{q}$ the wave vector. Expressing the electric field $\vec{E}$ in Ohm's law (3.57) through the electric potential V with the help of (3.59) and inserting the resulting expression for the current $\vec{J}$ in the continuity equation (3.58), the charge density ρ can be written as

Charge Density

$$\rho = \frac{\vec{q} \cdot \vec{J}}{\omega} = \frac{\bar{\sigma}}{\omega}\vec{q} \cdot \vec{E} = -i\frac{\bar{\sigma}q^2}{\omega}V. \tag{3.60}$$

For an external potential V the induced charge density is

Relation between Induced Charge Density and Polarization

$$\rho_{ind} = P^{(1)}(\vec{q}, \omega)V(\vec{q}, \omega) \tag{3.61}$$

where $P^{(1)}(\vec{q}, \omega)$ describes the dynamical polarization.

Comparing the two equations (3.60) and (3.61) one easily finds the relation between the dynamical polarization $P^{(1)}(\vec{q}, \omega)$ and the optical conductivity $\bar{\sigma}$

Relation between Dynamical Polarization and Optical Conductivity

$$P^{(1)}(\vec{q}, \omega) = -i\frac{\bar{\sigma}q^2}{\omega}. \tag{3.62}$$

The dynamical polarization is further related to the dielectric function via

Dielectric Function

$$\epsilon_r = 1 - V(q)P^{(1)}(\vec{q}, \omega). \tag{3.63}$$

As we are looking for a relation in 2 dimensions, we have to use the expression for the 2D electric potential, which is different form the one in 3 dimensions:

Electric Potential in 3D and 2D

$$\text{3D:} \quad V(q) = \frac{1}{\epsilon_0 q^2} \tag{3.64}$$

$$\text{2D:} \quad V(q) = \frac{1}{2\epsilon_0 q} \tag{3.65}$$

Hence, in 2 dimensions we find the following relations between $\bar{\sigma}_{2D}$ and ϵ_r

Relations between $\bar{\sigma}_{2D}$ and ϵ_r in 2D

$$P^{(1)}(\vec{q}, \omega) = -2\epsilon_0 q(\epsilon_r - 1) = -i\frac{\bar{\sigma}_{2D} q^2}{\omega} \tag{3.66}$$

$$\bar{\sigma}_{2D} = \frac{\omega}{iq^2} 2\epsilon_0 q(\epsilon_r - 1) = -i\frac{2\epsilon_0 \omega}{q}(\epsilon_r - 1) \tag{3.67}$$

3.3. Permittivity of T.I.s (2D free massless Dirac electrons)

We begin this section by solving the eigenvalue problem for a 2 dimensional system of free, massless Dirac electrons, before calculating the band overlap of these wave functions in 3.3.2, which is needed to derive the polarization function in 3.3.3. Section 3.3.3 is subdivided into the main parts of the calculation of the polarization function.

3.3.1. 2D free massless Dirac electron System EV

A 2D system of free, massless Dirac electrons can be described with the following Hamilton operator [23]:

Hamilton Operator for Free Massless Dirac Electrons

$$H = \hbar v_F \vec{\sigma} \cdot \vec{k} \tag{3.68}$$

with the reduced Planck constant $\hbar$, the Fermi velocity v_F and $\vec{\sigma} = (\sigma^x, \sigma^y)$ the vector of Pauli matrixes

Pauli Matrixes

$$\begin{aligned} \sigma^x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma^y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma^z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \tag{3.69}$$

where σ^z is not needed in our calculation and just given explicitly for completeness.

The Hamilton can therefore be rewritten as

$$\begin{aligned} H &= \hbar v_F \left[\begin{pmatrix} \sigma^x \\ \sigma^y \end{pmatrix} \cdot \begin{pmatrix} k_x \\ k_y \end{pmatrix} \right] = \hbar v_F \left(\sigma^x k_x + \sigma^y k_y \right) = \\ &= \hbar v_F \left[\begin{pmatrix} 0 & k_x \\ k_x & 0 \end{pmatrix} + \begin{pmatrix} 0 & -ik_y \\ ik_y & 0 \end{pmatrix} \right] = \\ &= \hbar v_F \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} . \end{aligned} \tag{3.70}$$

Switching to polar coordinates with the transformation rules

$$k = \sqrt{k_x^2 + k_y^2} \tag{3.71}$$

and

$$\phi = \arctan \left(\frac{k_y}{k_x} \right) \tag{3.72}$$

we get

$$H = \hbar v_F k \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} . \tag{3.73}$$

As was shown in chapter 2.3, in order to calculate the dielectric function describing the response of materials to external fields, we have to know the eigenenergies and eigenstates of a system. We therefore have to use the given Hamiltonian to solve the eigenvalue equation

Eigenvalue Equation

$$H\Psi_k = E\Psi_k \tag{3.74}$$

to obtain the eigenfunctions Ψ_k and eigenenergies E of our system:

$$\hbar v_F k \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \tag{3.75}$$

$$\Rightarrow \lambda^2 - (\hbar v_F k)^2 \stackrel{!}{=} 0 \Rightarrow \lambda \pm \hbar v_F k \tag{3.76}$$

As eigenfunctions for their respective eigenvalues (EV) we find:

EV: $+\hbar v_F k$:

$$\begin{pmatrix} -\hbar v_F k & \hbar v_F k e^{-i\phi} \\ \hbar v_F k e^{i\phi} & -\hbar v_F k \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{3.77}$$

$$\Rightarrow -\hbar v_F k c_1 + \hbar v_F k e^{i\phi} c_2 = 0 \tag{3.78}$$

$$\Rightarrow EF : \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} \tag{3.79}$$

EV: $-\hbar v_F k$:

$$\Rightarrow EF : \begin{pmatrix} e^{-i\phi} \\ -1 \end{pmatrix} \tag{3.80}$$

Eigenfunctions

$$\Rightarrow \quad |k, s = -1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ -1 \end{pmatrix}, \quad |k, s = +1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi} \\ 1 \end{pmatrix} \tag{3.81}$$

which can be combined to

Compact Eigenfunctions

$$\vec{F}_{s\vec{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi_{\vec{k}}} \\ s \end{pmatrix} \tag{3.82}$$

where $s = -1$ denotes the valence band and $s = +1$ the conduction band.

3.3.2. Overlap

A characteristic difference between the polarization of an ordinary 2DEG and an electron gas made of free massless Dirac electrons is the appearance of the band overlap of the wave functions.

To compute this overlap we find:

$$\begin{aligned}
\left|\vec{F}^{\dagger}_{s\vec{k}} \cdot \vec{F}_{s'\vec{k}+\vec{q}}\right|^2 &= \left|\frac{1}{2}\left(e^{i\phi_{\vec{k}}}, s\right) \cdot \begin{pmatrix} e^{i\phi_{\vec{k}+\vec{q}}} \\ s' \end{pmatrix}\right|^2 = \\
&= \frac{1}{4}\left|e^{i(\phi_{\vec{k}}-\phi_{\vec{k}+\vec{q}})} + ss'\right|^2 = \left\{\phi_{\vec{k}} - \phi_{\vec{k}+\vec{q}} \equiv \phi_{kk'}\right\} = \\
&= \frac{1}{4}\left(e^{i\phi_{kk'}} + ss'\right)\left(e^{-i\phi_{kk'}} + ss'\right) = \\
&= \frac{1}{4}\left[1 + ss'\left(e^{i\phi_{kk'}} + e^{-i\phi_{kk'}}\right) + (ss')^2\right] = \{s = \pm 1\} = \\
&= \frac{1}{4}\left(1 + 2ss'\cos(\phi_{kk'}) + 1\right) = \\
&= \frac{1 + ss'\cos(\phi_{kk'})}{2}.
\end{aligned} \tag{3.83}$$

with

$$\cos(\phi_{kk'}) = \frac{\vec{k}(\vec{k}+\vec{q})}{|\vec{k}||\vec{k}+\vec{q}|} = \frac{k^2 + kq\cos(\theta)}{k\sqrt{k^2+q^2+2kq\cos(\theta)}}. \tag{3.84}$$

ϕ is the angle between $\vec{k}$ and $\vec{k}+\vec{q}$, and θ is defined as the angle between $\vec{k}$ and $\vec{q}$ connected at their initial points. We get

Overlap

$$\left|\vec{F}^{\dagger}_{s\vec{k}} \cdot \vec{F}_{s'\vec{k}+\vec{q}}\right|^2 = \frac{1}{2}\left(1 + \frac{k^2 + kq\cos(\theta)}{k\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \equiv f^{ss'}(\vec{k},\vec{q}) \tag{3.85}$$

3.3.3. Polarization

In the previous two subsections of chapter 3 we have derived all quantities needed to calculate the polarization of a two dimensional gas of free, massless Dirac electrons. [13, 31] As derived in chapter 2.3, the response of an electronic system to an external electric potential in form of the polarization function is given by

Polarization

$$P(\vec{q},\omega) = \frac{g_s g_v}{4\pi^2} \int \sum_{s,s'=\pm} \frac{n_F\left(E^s(k)\right) - n_F\left(E^{s'}(|\vec{k}+\vec{q}|)\right)}{\hbar\omega + E^s(k) - E^{s'}(|\vec{k}+\vec{q}|) + \mathrm{i}0} f^{\mathrm{ss}'}(\vec{k},\vec{q}) d^2k \tag{3.86}$$

with g_s, g_v the spin and valley degeneracy (both 1 in our case) and the Fermi function

Fermi Function

$$n_F\left(E^s\right) = \frac{1}{e^{\beta E}+1}, \tag{3.87}$$

describing the distribution of the electrons in dependence of their energies. The energies are given by the dispersion relation

Eigenenergies

$$E^{\pm}(k) = \pm\hbar v_F k \tag{3.88}$$

as found in 3.3.1 as the eigenenergies of our system. For an excited state with wave vector $\vec{k}+\vec{q}$ this becomes

$$E^{\pm}(|\vec{k}+\vec{q}|) = \pm\hbar v_F \sqrt{k^2+q^2-2kq\cos(\phi)}. \tag{3.89}$$

ϕ is the angle between $\vec{k}$ and $\vec{q}$ when connecting the initial point of $\vec{q}$ to the terminal point of $\vec{k}$. θ in the integral is defined as the angle between $\vec{k}$ and $\vec{q}$ connected at their initial points. We therefore have the relation $\phi = \pi$ - θ between the two angles.

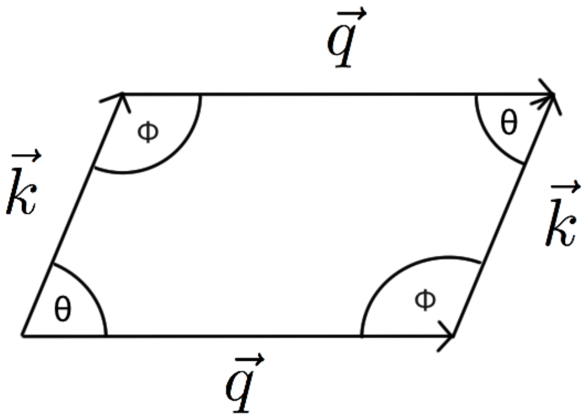

Figure 3.2.: Definition of wavevectors and angles used in our calculations. θ is the angle between $\vec{k}$ and $\vec{q}$ connected at their initial points, ϕ is the angle between $\vec{k}$ and $\vec{q}$ when connecting the initial point of $\vec{q}$ to the terminal point of $\vec{k}$. The two angles are related via $\phi = \pi$ - θ.

As the cosine is a symmetric and periodic function with a period of 2π:

$$\cos(\pi - \theta) = \cos(\theta - \pi) = -\cos(\theta), \tag{3.90}$$

we find for the square root in (3.89), remembering (3.90) and $\phi = \pi$ - θ:

$$\Rightarrow k^2 + q^2 - 2kq\cos(\phi) = k^2 + q^2 + 2kq\cos(\theta) \tag{3.91}$$

The eigenenergies can therewith be rewritten as

$$E^{\pm}(|\vec{k} + \vec{q}|) = \pm\hbar v_F \sqrt{k^2 + q^2 + 2kq\cos(\theta)} \tag{3.92}$$

As calculated in 3.3.2, the overlap between initial and final state is

Overlap

$$f^{\mathrm{ss}'}(\vec{k},\vec{q}) = \frac{1}{2}\left(1 + \mathrm{ss}'\frac{k + q\cos(\theta)}{\sqrt{k^2 + 2kq\cos(\theta) + q^2}}\right). \tag{3.93}$$

We now make in the term $n_F(E^{s'}(|\vec{k}+\vec{q}|))$ a resummation of the form $\vec{k} \to -\vec{k} - \vec{q}$ that does not change $f^{\mathrm{ss}'}$:

$$\cos(\theta) = \frac{\vec{k}(\vec{k}+\vec{q})}{k|\vec{k}+\vec{q}|} \to \frac{(-\vec{k}-\vec{q})(-\vec{k})}{|-\vec{k}-\vec{q}||-\vec{k}|} = \cos(\theta) \tag{3.94}$$

Setting $g_s g_v = g$, we get

$$P(\vec{q},\omega) = \frac{g}{4\pi^2}\int \sum_{s,s'=\pm} f^{\mathrm{ss}'}(\vec{k},\vec{q}) n_F\left(E^s(k)\right) \left(\frac{1}{\hbar\omega + E^s(k) - E^{s'}(|\vec{k}+\vec{q}|) + \mathrm{i}0} - \frac{1}{\hbar\omega - E^s(k) + E^{s'}(|\vec{k}+\vec{q}|) + \mathrm{i}0}\right) d^2k \tag{3.95}$$

where we changed in the second term $s \to s'$ and used $E^s(k) = E^s(-k)$.

We have to consider all physically possible excitations in (3.95). As the cone labeled with -1 (visualized by the lower cone in figure 3.3), representing the lower band, is full and the cone labeled with $+1$ (visualized by the upper cone in figure 3.3), representing the upper band is partly filled, there exist two types of excitations. On the one hand we can get intraband transitions in the upper band from the occupied states to empty ones, on the other hand, if the excitation energy is large enough, there also exist interband transitions from the full cone underneath to the empty part of the upper one. This circumstance is illustrated in figure 3.3.

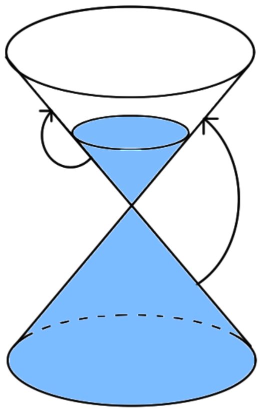

Figure 3.3.: Illustration of all possible excitations in the Dirac cone for $\mu > 0$. There exist intra- and interband excitations depending on the excitation energy.

In order to ease the calculation, we split this physically correct picture into an equivalent, but mathematical more comfortable one. As shown in figure 3.4, the excitations in the Dirac cone can be divided into three parts:

- for $\mu = 0$ we only have interband transitions from the full cone underneath to the empty upper cone
- for $\mu > 0$ we have to add intraband transitions in the upper band
- and we must subtract interband contributions from the cone beneath to the upper cone where the final state is already occupied

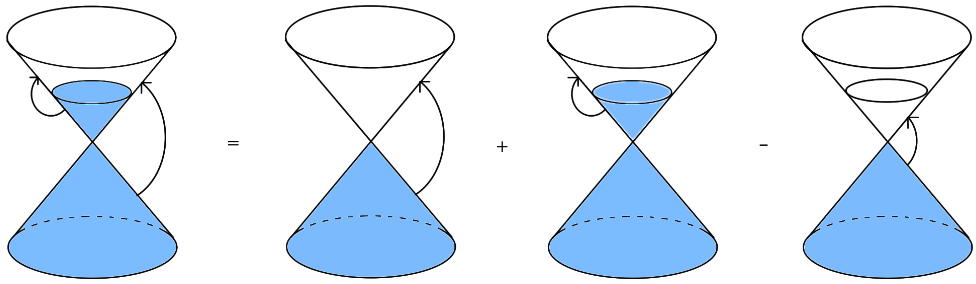

Figure 3.4.: All the possible excitations in the Dirac cone for $\mu > 0$ (left) can be (mathematically) split into three parts (from left to right): interband transitions for $\mu = 0$, intraband transitions in the upper band for $\mu > 0$ and a negative contribution stemming from forbidden transitions for $\mu > 0$ that we ignored when considering interband transitions by setting $\mu = 0$.

Looking at figure 3.5, it becomes apparent, that the contribution of the last cone as seen in figure 3.4, which has to be subtracted, can be substituted by adding its inverse.

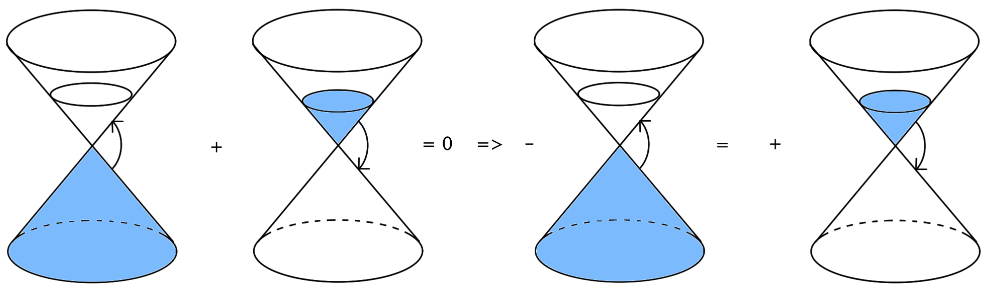

Figure 3.5.: The contribution from the last cone in figure 3.4 can be compensated by its inverse. We can therefore replace the subtraction of the last cone by the addition of its inverse.

We can therefore split figure 3.3 as follows:

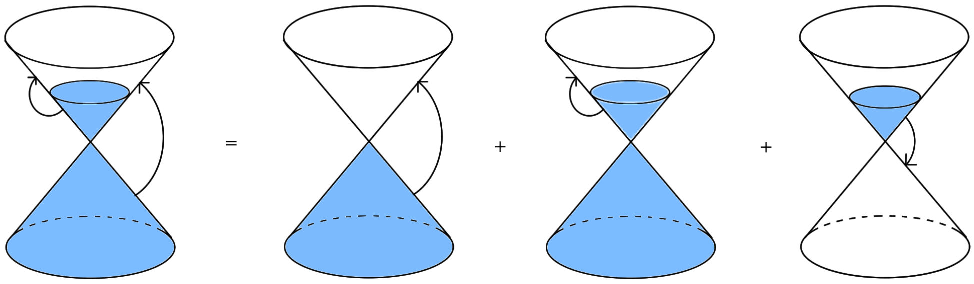

Figure 3.6.: All the possible excitations in the Dirac cone for $\mu > 0$ (left) can be (mathematically) split into three parts (from left to right): interband transitions for $\mu = 0$, intraband transitions in the upper band for $\mu > 0$ and a contribution stemming from forbidden transitions for $\mu > 0$ that we ignored when considering interband transitions by setting $\mu = 0$.

Lets now write down the three integrals explicitly:

For $\mu = 0$ we only have interband transitions from the full cone underneath to the empty upper cone. We have to integrate over all possible wave vectors of the initial states, thus $0 \leq k < \infty$. As we only have transitions from the valence band to the conduction band, we set $s = -1, s' = 1$.

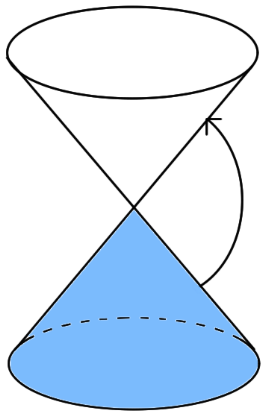

Figure 3.7.: Illustration of all possible excitations in the Dirac cone for $\mu = 0$. There only exist interband excitations.

The polarization thus reads : (μ = 0, s = -1, s' = 1)

Polarization for μ = 0, s = -1, s' = 1

$$P^0(\vec{q},\omega) = \frac{g}{4\pi^2\hbar}\int_{k<\Lambda} f^-(\vec{k},\vec{q}) \tag{3.96}$$

$$\left(\frac{1}{\omega - v_F(k+|\vec{k}+\vec{q}|)+\mathrm{i}0} - \frac{1}{\omega + v_F(k+|\vec{k}+\vec{q}|)+\mathrm{i}0}\right) d^2k \tag{3.97}$$

$$= -\chi^-_\Lambda(\vec{q},\omega) \text{ for } \Lambda \to \infty \tag{3.98}$$

For $\mu > 0$ we get two additional contributions:

Firstly, we have to add intraband transitions in the upper band, thus $s = s' = 1$ and integrate over all possible wave vectors of the initial states, in this case $0 \leq k < k_F$.

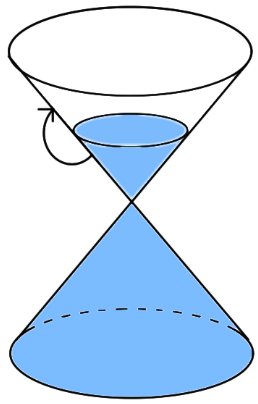

Figure 3.8.: Illustration of possible intraband excitations in the Dirac cone for $\mu > 0$.

Polarization for $\mu = 0$, s = s' = 1

$$\Delta \mathrm{P}^{+}(\vec{q},\omega) = \frac{g}{4\pi^2\hbar}\int_{k<k_F} f^{+}(\vec{k},\vec{q})$$
$$\left(\frac{1}{\omega + v_F(k - |\vec{k}+\vec{q}|) + \mathrm{i}0} - \frac{1}{\omega - v_F(k - |\vec{k}+\vec{q}|) + \mathrm{i}0}\right) d^2k = \chi^{+}_{k_F}(\vec{q},\omega) \quad (3.99)$$

Secondly, we must subtract interband contributions from the cone beneath to the upper cone where the final state $E^{s'}(|\vec{k}+\vec{q}|) < \mu$. As was shown above, this is equivalent to adding a term with $s = -1, s' = 1$ (where s and s' where interchanged in the equation) and using $0 \leq k < k_F$ as boundaries.

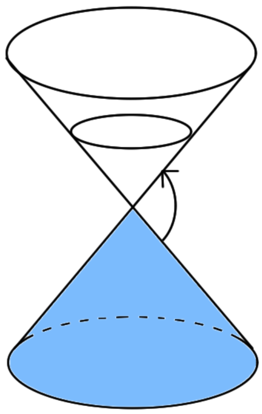

Figure 3.9.: Illustration of the contribution stemming from forbidden transitions for $\mu > 0$ that we ignored when considering interband transitions by setting $\mu = 0$, and thus have to subtract afterwards.

Resummation in the first term of the equation describing the polarization gives

$$P(\vec{q},\omega) = \frac{g}{4\pi^2} \int \sum_{s,s'=\pm} f^{\mathrm{ss}'}(\vec{k},\vec{q}) n_F(E^{s'}(|\vec{k}+\vec{q}|)) \\ \left(\frac{1}{\hbar\omega - E^s(k) + E^{s'}(|\vec{k}+\vec{q}|) + \mathrm{i}0} - \frac{1}{\hbar\omega + E^s(k) - E^{s'}(|\vec{k}+\vec{q}|) + \mathrm{i}0} \right) d^2k \quad (3.100)$$

For s = -1, s' = 1 we get

Polarization for $\mu > 0$, s = -1, s' = 1

$$\Delta \mathrm{P}^{-}(\vec{q},\omega) = \frac{g}{4\pi^2\hbar}\int_{k<k_F} f^{-}(\vec{k},\vec{q})$$
$$\left(\frac{1}{\omega + v_F(k+|\vec{k}+\vec{q}|)+\mathrm{i}0} - \frac{1}{\omega - v_F(k+|\vec{k}+\vec{q}|)+\mathrm{i}0}\right) d^2k = \chi^{-}_{k_F}(\vec{q},\omega) \tag{3.101}$$

Putting all contributions together, we find that the polarization is given by

Polarization

$$\begin{aligned} P(\vec{q},\omega) &= P^0(\vec{q},\omega) + \Delta \mathrm{P}^{+}(\vec{q},\omega) + \Delta \mathrm{P}^{-}(\vec{q},\omega) \\ &= -\chi_{\Lambda\to\infty}{}^{-}(\vec{q},\omega) + \chi_{k_F}{}^{+}(\vec{q},\omega) + \chi^{-}_{k_F}(\vec{q},\omega) \end{aligned} \tag{3.102}$$

Before explicitly evaluating these integrals, we simplify our notation by setting $v_F = \hbar = 1$, so that $\mu = k_F$ during this calculation. We further introduce the parameters α and β that will help us attribute the individual terms in the integrals to a general form.

We have to solve the following integrals for P^0 and ΔP^- with $\tau = \Lambda = \infty$ for P^0 and with $\tau = \mu$ for ΔP^-:

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 - \frac{k + q\cos(\theta)}{\sqrt{k^2 + q^2 + 2kq\cos(\theta)}}\right) \frac{1}{\left(\omega - \left(k + \sqrt{k^2 + q^2 + 2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \tag{3.103}$$

and

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 - \frac{k + q\cos(\theta)}{\sqrt{k^2 + q^2 + 2kq\cos(\theta)}}\right) \frac{1}{\left(\omega + \left(k + \sqrt{k^2 + q^2 + 2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \tag{3.104}$$

which can be combined to

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 - \frac{k + q\cos(\theta)}{\sqrt{k^2 + q^2 + 2kq\cos(\theta)}}\right) \frac{1}{\left(\omega + \alpha\left(k + \sqrt{k^2 + q^2 + 2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \tag{3.105}$$

with $\alpha = -1$ for the first and $\alpha = +1$ for the second integral.

For ΔP^{+} we have to solve the following integrals for $\tau = \mu$:

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 + \frac{k + q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega + \left(k - \sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) + \mathrm{i}0}\, d\theta dk \quad (3.106)$$

and

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 + \frac{k + q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega - \left(k - \sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \quad (3.107)$$

which can be combined to

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 + \frac{k + q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega + \alpha\left(k - \sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \quad (3.108)$$

with $\alpha = 1$ for the first and $\alpha = -1$ for the second integral.

Finally we can combine all 4 integrals to

$$\int_0^\tau k \int_0^{2\pi} \frac{1}{2}\left(1 + \beta\frac{k + q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega + \alpha\left(k - \beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) + \mathrm{i}0} d\theta dk \quad (3.109)$$

with $\beta = -1$ for P^0 and ΔP^- and $\beta = 1$ for ΔP^+.

We find the general expression for the integrals we have to solve to be:

Polarization Function

$$\chi_D{}^{\beta}(\vec{q},\omega) = \frac{g}{4\pi^2\hbar}\int_{k\leq D}\sum_{\alpha=\pm}\frac{\alpha f^{\beta}(\vec{k},\vec{q})}{\omega+\alpha \mathrm{v}_F(k-\beta|\vec{k}+\vec{q}|)+\mathrm{i}0}d^2k \tag{3.110}$$

In the following we present some major steps of the calculation and refer to the appendix for an extensive derivation. The complex calculation will be split into two main parts, one for the imaginary part and one for the real part. Each part will further be subdivided into $\theta-$ and $k-$ integration and the solutions will be given in separate regions of the $q-\omega-$plane. A general solution therefrom is given in chapter 4. With the exception of the introduction of the different regions of the $q-\omega-$plane, which is visualized in figure 3.10 and to that will be referred later on, the remaining part of chapter 3 is mainly algebra.

3.3.3.1. Imaginary Part

Using the identity

Identity

$$\frac{1}{x \pm i0} = P\frac{1}{x} \mp i\pi\delta(x) \tag{3.111}$$

we get for the imaginary part :

Imaginary Part of the Polarization

$$-\frac{g}{4\pi}\int_0^{\tau} k \sum_{\alpha=\pm 1} \alpha \int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) d\theta dk \tag{3.112}$$

3.3.3.1.1. θ-Integration Calculation of the θ - integral:

θ - integral of the Imaginary Part of the Polarization

$$k\int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) d\theta \tag{3.113}$$

The only contribution we get from this integral is for

$$\delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)=1. \tag{3.114}$$

Therefore we have to find all zeros of

$$\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right) \tag{3.115}$$

regarding to θ.

We find (with the exceptions $\{\alpha=1,\beta=-1\}$, $\{\alpha=-1,\beta=1$ for $0<q<\omega$ and $\frac{1}{2}(-q+\omega)\leq k\leq\frac{q+\omega}{2}\}$, $\{\alpha=-1,\beta=-1,q>\omega$ and $k\geq\frac{q+\omega}{2}\}$)

$$\theta=-\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{3.116}$$

and

$$\theta=\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{3.117}$$

As the arccos is only defined between (-1, 1)

$$1\geq\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\geq-1 \tag{3.118}$$

we get θ-functions of the form

$$\theta(\alpha)\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right) \tag{3.119}$$

for $\alpha=1$ and

$$\theta\left(-\alpha\right)\left(\theta\left(\omega-q\right)\left(\theta\left(\frac{\omega+q}{2}-k\right)-\theta\left(\frac{\omega-q}{2}-k\right)\right)+\theta\left(q-\omega\right)\theta\left(k-\frac{q-\alpha\omega}{2}\right)\right) \tag{3.120}$$

for $\alpha = -1$.

This adds up to:

$\boldsymbol{\theta}$−Functions

$$\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right)+\theta(-\alpha)\left(\theta(\omega-q)\left(\theta\left(\frac{\omega+q}{2}-k\right)-\theta\left(\frac{\omega-q}{2}-k\right)\right)\right) \tag{3.121}$$

With the substitution rule

Substitution Rule

$$\delta(g(x))=\sum_{x_i:g(x_i)=0}\frac{\delta\left(x-x_i\right)}{\left|g'\left(x_i\right)\right|} \tag{3.122}$$

with the sum over all zeros of the δ - function we get :

$$\frac{d}{d\theta}\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)=\frac{kq\alpha\beta\sin(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}} \tag{3.123}$$

which leads to

$$-\frac{kq\alpha\beta\sqrt{1-\frac{\left(q^2-\omega(2k\alpha+\omega)\right)^2}{4k^2q^2}}}{\sqrt{k^2+2k\alpha\omega+\omega^2}} \tag{3.124}$$

for

$$\theta=-\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{3.125}$$

and

$$\frac{kq\alpha\beta\sqrt{1-\frac{(q^2-\omega(2k\alpha+\omega))^2}{4k^2q^2}}}{\sqrt{k^2+2k\alpha\omega+\omega^2}} \tag{3.126}$$

for

$$\theta = \arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{3.127}$$

The absolute value for both solutions is the same. The δ - function can now be written as

$$\begin{aligned}
&\delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right) = \\
&\left|\frac{\sqrt{k^2+2k\alpha\omega+\omega^2}}{kq\alpha\beta\sqrt{1-\frac{(q^2-\omega(2k\alpha+\omega))^2}{4k^2q^2}}}\right| \\
&\left(\delta\left(\theta+\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right)\right)+\delta\left(\theta-\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right)\right)\right) \\
&\left(\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right)\right. \\
&\left.+\theta(-\alpha)\left(\theta(\omega-q)\left(\theta\left(\frac{\omega+q}{2}-k\right)-\theta\left(\frac{\omega-q}{2}-k\right)\right)\right)\right)
\end{aligned} \tag{3.128}$$

And the θ - integration yields :

Result of the θ Integartion of the Imaginary Part

$$\begin{aligned}
&\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta((q-\omega))\theta\left(k-\frac{q-\omega}{2}\right)+ \\
&\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right)+ \\
&\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right),
\end{aligned} \tag{3.129}$$

which is always real.

3.3.3.1.2. k-Integration Defining

Definition for Imaginary Part

$$I^{\alpha\beta}(k,q,\omega) = \sqrt{\frac{(2\alpha\mathrm{k}+\omega)^2 - q^2}{(q^2-\omega^2)}}\left(\theta(\beta)\theta(q-\omega)\theta\left(k - \frac{q-\alpha\omega}{2}\right) + \theta(-\beta)\theta(\omega-q)\theta(-\alpha)\left(\theta\left(-k+\frac{q+\omega}{2}\right) - \theta\left(-k+\frac{-q+\omega}{2}\right)\right)\right), \quad (3.130)$$

we can rewrite the imaginary part of the functions $\chi_D^\beta(q,\omega)$ as

Imaginary Part of $\chi_D^\beta(q,\omega)$

$$\mathrm{Im}\chi_D^\beta(q,\omega) = -\frac{g}{4\pi}\int_0^\tau \sum_{\alpha=\pm 1} \alpha I^{\alpha\beta}(k,q,\omega)dk \quad (3.131)$$

For $\mu = 0$ (interband transitions from the full cone underneath to the empty upper cone) we get from the k - integration (Fermi function equal 1 in the cone beneath and zero in the upper cone)

$\mu = 0$ Contribution to the Imaginary Part of the Polarization

$$\begin{aligned}
&\mathrm{Im}P^0(\vec{q},\omega) = -\mathrm{Im}{X_\Lambda}^-(\vec{q},\omega) = \frac{g}{4\pi}\int_0^{\Lambda\to\infty}\sum_{\alpha=\pm1}\alpha \mathrm{I}^{\alpha-}dk \\
&= -\frac{g}{4\pi}\int_0^{\infty}\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta(\omega-q)\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk \\
&= -\frac{gq^2\theta(-q+\omega)}{16\sqrt{-q^2+\omega^2}}
\end{aligned} \tag{3.132}$$

For $\mu > 0$ we get two additional contributions:

(i) s = s' = 1 (intraband transitions in the upper band)
(ii) interband contributions from the cone beneath to the upper cone where the final state $E^{s'}(|\vec{k}+\vec{q}|) < \mu$.

$$\begin{aligned}
\mathrm{Im}\Delta\mathrm{P}^1(\vec{q},\omega) &= \mathrm{Im}\Delta\mathrm{P}^+(\vec{q},\omega) + \mathrm{Im}\Delta\mathrm{P}^-(\vec{q},\omega) \\
&= \mathrm{Im}{\chi_{k_F}}^+(q,\omega) + \mathrm{Im}{\chi_{k_F}}^-(q,\omega) \\
&= -\frac{g}{4\pi}\int_0^{\mu}\sum_{\alpha,\beta=\pm1}\alpha \mathrm{I}^{\alpha\beta}dk
\end{aligned} \tag{3.133}$$

We have to solve the integral

k-Integration of Imaginary Part

$$
\begin{aligned}
&-\frac{g}{4\pi}\int_0^{\mu}\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right) \\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right) \\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk
\end{aligned}
\tag{3.134}
$$

The θ-functions divide our solutions in 6 regions that are limited by the straight lines $\omega = v_F q$, $\omega = v_F q - 2\mu$ and $\omega = 2\mu - v_F q$.

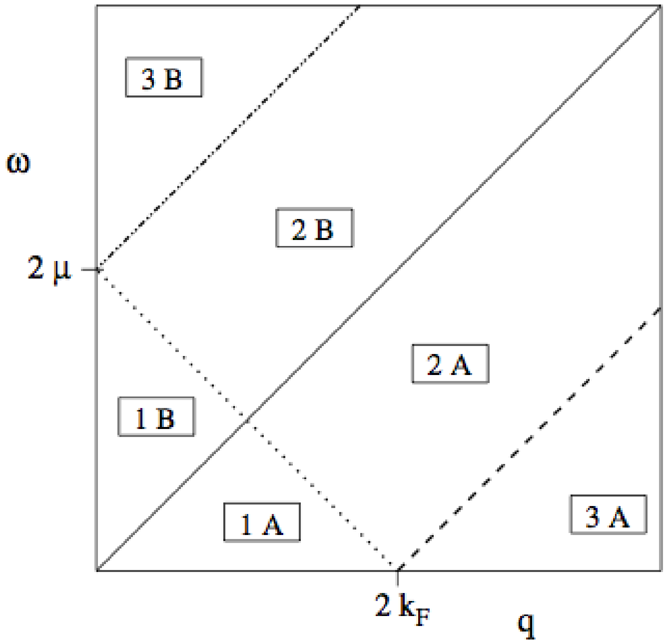

Figure 3.10.: Display of the different regions originating from the θ-functions. The regions are limited by the straight lines $\omega = v_F q$, $\omega = v_F q - 2\mu$ and $\omega = 2\mu - v_F q$. We note that only in region 1B we find $P^{(1)}(q,\omega) = 0$ and can hence expect to find stable plasmons. [31]

Regions Originating from θ Functions

$$\begin{aligned}
1A: &\quad (0 < \text{q} < 2\ \mu,\ \omega < \text{q},\ \omega < \text{-q} + 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)\\
2A: &\quad (\omega < \text{q},\ \omega > \text{q - } 2\ \mu,\ \omega > \text{-q} + 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)\\
3A: &\quad (\text{q} > 2\ \mu,\ \omega < \text{q - } 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)\\
1B: &\quad (0 < \text{q} < \mu,\ \omega > \text{q},\ \omega < \text{-q} + 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)\\
2B: &\quad (\omega > \text{q},\ \omega < \text{q} + 2\ \mu,\ \omega > \text{-q} + 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)\\
3B: &\quad (\omega > \text{q} + 2\ \mu,\ \omega > 0,\ \text{q} > 0,\ \mu > 0)
\end{aligned} \tag{3.135}$$

Imaginary part in area 1A is given by:

Imaginary Part of the Polarization in Area 1A

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2} \right.$$
$$\left. -\operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right) - \left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} + \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right) \tag{3.136}$$

Imaginary part in area 2A is given by:

Imaginary Part of the Polarization in Area 2A

$$= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} - \ln\left(\frac{2\mu+\omega}{q} + \sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right) \tag{3.137}$$

Imaginary part in area 3A is 0.
Imaginary part in area 1B is given by:

Imaginary Part of the Polarization in Area 1B

$$= \frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \tag{3.138}$$

Imaginary part in area 2B is given by:

Imaginary Part of the Polarization in Area 2B

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}}\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\frac{-2\mu+\omega}{q}\right)\right) \tag{3.139}$$

Imaginary part in area 3B is 0.

3.3.3.2. Real Part

Lets now calculate the real part of:

$$\int_0^{\tau} k \int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)+\mathrm{i}0} d\theta dk \tag{3.140}$$

Using the identity

Identity

$$\frac{1}{x \pm i0} = P\frac{1}{x} \mp i\pi\delta(x) \tag{3.141}$$

we get for the real part :

Real Part of the Polarization

$$\frac{g}{4\pi^2}\int_0^\tau k\sum_{\alpha=\pm1}\alpha\int_0^{2\pi}\frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right)$$
$$\frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)}d\theta dk \quad (3.142)$$

3.3.3.2.1. θ-Integration Calculation of the θ - integral:

θ Integarl of the Real Part of the Polarization Function

$$\alpha\int_0^{2\pi}\frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right)$$
$$\frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)}d\theta \quad (3.143)$$

The integral can be simplified to:

$$\alpha\int_0^{2\pi}\frac{2k+\alpha\omega+q\cos(\theta)}{(k+\alpha\omega)^2-(k^2+q^2+2kq\cos(\theta))}\,d\theta \quad (3.144)$$

We get for $\alpha=1$:

$$\alpha\int_0^{2\pi}\frac{2k+\omega+q\cos(\theta)}{(\omega+k)^2-(k^2+q^2+2kq\cos(\theta))}\,d\theta = \quad (3.145)$$

$$\left(-\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right) \quad (3.146)$$

and for $\alpha = -1$:

$$\alpha \int_0^{2\pi} \frac{2k - \omega + q\cos(\theta)}{(\omega - k)^2 - (k^2 + q^2 + 2kq\cos(\theta))}\, d\theta = \tag{3.147}$$

$$= \left(-\frac{\pi}{k} + \frac{\pi\sqrt{\frac{(-2k+\omega)^2 - q^2}{\omega^2 - q^2}}}{k}\right)$$
$$\left(\theta(\omega - q)\theta\left(\frac{-q+\omega}{2} - k\right) + \theta(q - \omega)\theta\left(\frac{q+\omega}{2} - k\right)\right) +$$
$$\left(-\frac{\pi}{k} - \frac{\pi\sqrt{\frac{(-2k+\omega)^2 - q^2}{\omega^2 - q^2}}}{k}\theta(\omega - q)\theta\left(k - \frac{q+\omega}{2}\right)\right) \tag{3.148}$$

All together we arrive at (where we already multiplied with k in the integrand):

Result of the θ Integarl of the Real Part of the Polarization Function

$$\left(-\pi + \pi\sqrt{\frac{(2k+\omega)^2 - q^2}{\omega^2 - q^2}}\right)\left(\theta(q - \omega)\theta\left(\frac{q-\omega}{2} - k\right) + \theta(\omega - q)\right) +$$
$$\left(-\pi + \pi\sqrt{\frac{(-2k+\omega)^2 - q^2}{\omega^2 - q^2}}\right)$$
$$\left(\theta(\omega - q)\theta\left(\frac{-q+\omega}{2} - k\right) + \theta(q - \omega)\theta\left(\frac{q+\omega}{2} - k\right)\right) +$$
$$\left(-\pi - \pi\sqrt{\frac{(-2k+\omega)^2 - q^2}{\omega^2 - q^2}}\right)\theta(\omega - q)\theta\left(k - \frac{q+\omega}{2}\right) \tag{3.149}$$

3.3.3.2.2. k-Integration For $\mu = 0$ (interband transitions from the full cone underneath to the empty upper cone) we get using the Kramers - Kronig relation (Fermi function equal 1 in the cone beneath and zero in the upper cone)

$\mu = 0$ Contribution to the Real Part of the Polarization

$$\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega' \left(-\frac{gq^2\theta(-q+\omega')}{16\sqrt{-q^2+\omega'^2}}\frac{1}{\omega'-\omega}\right) = -\frac{gq^2\left(\arccos\left(-\frac{\omega}{q}\right)\right)}{16\pi\sqrt{q^2-\omega^2}}\theta(q-\omega) \quad (3.150)$$

For $\mu > 0$ we get two additional contributions:

(i) s = s' = 1 (intraband transitions in the upper band)
(ii) interband contributions from the cone beneath to the upper cone where the final state $E^{s'}(|\vec{k}+\vec{q}|) < \mu$.
$-\pi$ is treated separately - it yields $-\frac{g\mu}{2\pi}$ for every region, we just have to integrate

k-Integration of Real Part

$$\left(\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)+$$
$$\left(\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)+$$
$$\left(-\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right) \quad (3.151)$$

Again we use our 6 regions defined previously to determine the solutions of the k-integration in every area separately.

Real part in area 1A is given by:

Real Part of the Polarization in Area 1A

$$= \frac{gq^2}{16\sqrt{q^2 - \omega^2}} \tag{3.152}$$

Real part in area 2A is given by:

Real Part of the Polarization in Area 2A

$$= \frac{gq^2}{16\pi\sqrt{q^2 - \omega^2}} \left(-\left(\frac{\omega - 2\mu}{q}\right)\sqrt{1 - \left(\frac{\omega - 2\mu}{q}\right)^2} + \arccos\left(\left(\frac{\omega - 2\mu}{q}\right)\right)\right), \tag{3.153}$$

for $\left|\frac{\omega-2\mu}{q}\right| < 1$

Real part in area 3A is given by

Real Part of the Polarization in Area 3A

$$\begin{aligned} &= \frac{gq^2}{16\pi\sqrt{q^2 - \omega^2}} \\ &\left(\left(-\left(\frac{\omega - 2\mu}{q}\right)\sqrt{1 - \left(\frac{\omega - 2\mu}{q}\right)^2} + \arccos\left(\frac{\omega - 2\mu}{q}\right)\right)\right. \\ &+ \left.\left(\left(\frac{2\mu + \omega}{q}\right)\sqrt{1 - \left(\frac{2\mu + \omega}{q}\right)^2} - \arccos\left(\frac{2\mu + \omega}{q}\right)\right)\right), \end{aligned} \tag{3.154}$$

for $\left|\frac{\omega-2\mu}{q}\right| < 1$.

Real part in area 1B is given by

Real Part of the Polarization in Area 1B

$$= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \left(-\left(\frac{2\mu-\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2} + \operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right) + \left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right) \tag{3.155}$$

Real part in area 2B is given by

Real Part of the Polarization in Area 2B

$$= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{\left(-1+\left(\frac{2\mu+\omega}{q}\right)^2\right)} - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right) \tag{3.156}$$

Real part in area 3B is given by

Real Part of the Polarization in Area 3B

$$= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \left(\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{\omega-2\mu}{q}\right)^2} - \operatorname{arccosh}\left(\frac{\omega-2\mu}{q}\right)\right) - \left(\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right)\right) \tag{3.157}$$

4. Results

In this chapter the main results of this thesis are presented. We start with a compact solution for the polarization function of 2D free massless Dirac electrons in 4.1. Further their 2D dielectric function and 2D conductivity will be given explicitly in 4.2. Finally, in section 4.3, we will prove the existence and discuss the topic of this whole work, plasmons in topological insulators.

4.1. Polarisation Function of 2D free massless Dirac Electrons

In order to present the results found in chapter 3.3 in a more compact form, we introduce the following real-valued functions:

Real Functions

$$\begin{aligned} f(q,\omega) &= \frac{g}{16\pi}\frac{q^2}{\sqrt{|\omega^2-q^2|}} \\ G_>(x) &= x\sqrt{x^2-1}-\cosh^{-1}(x), \quad x>1, \\ G_<(x) &= x\sqrt{1-x^2}-\cos^{-1}(x), \quad |x|>1, \end{aligned} \tag{4.1}$$

and find for the imaginary part of $\Delta P^{(1)}$

Imaginary Part of $\Delta P^{(1)}$

$$\mathrm{Im}\Delta P^{(1)}(q,\omega) = f(q,\omega)\cdot\begin{cases} G_>\left(\frac{2\mu-\omega}{q}\right)-G_>\left(\frac{2\mu+\omega}{q}\right), & 1A \\ \pi, & 1B \\ -G_>\left(\frac{2\mu+\omega}{q}\right), & 2A \\ -G_<\left(\frac{\omega-2\mu}{q}\right), & 2B \\ 0, & 3A \\ 0, & 3B \end{cases} \tag{4.2}$$

and for the real part of $\Delta P^{(1)}$

Real Part of $\Delta P^{(1)}$

$$\mathrm{Re}\Delta P^{(1)}(q,\omega) = f(q,\omega)\cdot \begin{cases} \pi, & 1A \\ -G_>\left(\frac{2\mu-\omega}{q}\right) + G_>\left(\frac{2\mu+\omega}{q}\right), & 1B \\ -G_<\left(\frac{\omega-2\mu}{q}\right), & 2A \\ G_>\left(\frac{2\mu+\omega}{q}\right) & 2B \\ -G_<\left(\frac{\omega-2\mu}{q}\right) + G_<\left(\frac{2\mu+\omega}{q}\right), & 3A \\ G_>\left(\frac{2\mu+\omega}{q}\right) - G_>\left(\frac{\omega-2\mu}{q}\right), & 3B \end{cases} \tag{4.3}$$

To unify this even further, we note the following properties

Properties Between Logarithms and Trigonometric Functions

$$\begin{aligned} &\Theta(x-1)\cosh^{-1}(x) = \ln\left(x+\sqrt{x^2-1}\right), \\ &\Theta(1-x^2)\cos^{-1}(x) = -i\ln\left(x+i\sqrt{1-x^2}\right), \\ &\cos^{-1}(-x) = \pi - \cos^{-1}(x). \end{aligned} \tag{4.4}$$

Thus the single function $G(x) = x\sqrt{x^2-1} - \ln(x+\sqrt{x^2-1})$ can comprise the functions $G_>(x)$ and $G_<(x)$ where

Single Function

$$G(x) = \begin{cases} G_>(x), & x > 1 \\ iG_<(x) = -i[\pi + G_<(-x)], & |x| < 1. \end{cases} \tag{4.5}$$

We also define the complex function $F(q,\omega)$ with the property $f(q,\omega) = |F(q,\omega)|$. [31] With this functions the polarization $P^{(1)}(q,\omega)$ can be writing in the compact form

Compact Form of the Polarization $P^{(1)}(q,\omega)$

$$
\begin{aligned}
P^{(1)}(q,\omega) = &-i\pi\frac{F(q,\omega)}{\hbar^2 v_F^2} - \frac{g\mu}{2\pi\hbar^2 v_F^2} + \frac{F(q,\omega)}{\hbar^2 v_F^2}\cdot G\left(\frac{\hbar\omega + 2\mu}{\hbar v_F q}\right) \\
&- \frac{F(q,\omega)}{\hbar^2 v_F^2}\cdot\Theta\left(\frac{2\mu-\hbar\omega}{\hbar v_F q} - 1\right)\cdot\left(G\left(\frac{2\mu-\hbar\omega}{\hbar v_F q}\right) - i\pi\right) \\
&- \frac{F(q,\omega)}{\hbar^2 v_F^2}\cdot\Theta\left(\frac{\hbar\omega-2\mu}{\hbar v_F q} - 1\right)\cdot G\left(\frac{\hbar\omega-2\mu}{\hbar v_F q} - 1\right)
\end{aligned}
\tag{4.6}
$$

Inserting the functions $F(x)$ and $G(x)$ this expands to:

Expanded Form of the Polarization $P^{(1)}(q,\omega)$

$$
\begin{aligned}
P^{(1)}(q,\omega) = &-\frac{g\mu}{2\pi\hbar^2 v_F^2} - \frac{igq^2}{16\hbar\sqrt{\omega^2 - q^2 v_F^2}} - \frac{gq^2}{16\pi\hbar\sqrt{\omega^2 - q^2 v_F^2}}\cdot \\
&\Bigg\{\Theta\left(\frac{2\mu-\omega\hbar}{q\hbar v_F} - 1\right)\cdot \\
&\left[\frac{(2\mu-\omega\hbar)\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - i\pi\ln\left(\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu-\omega\hbar}{q\hbar v_F}\right)\right] \\
&-\Theta\left(\frac{\omega\hbar-2\mu}{q\hbar v_F} + 1\right)\cdot \\
&\left[\frac{(\omega\hbar-2\mu)\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{\omega\hbar-2\mu}{q\hbar v_F}\right)\right] + \\
&+\left(\frac{(2\mu+\omega\hbar)\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu+\omega\hbar}{q\hbar v_F}\right)\right)\Bigg\}
\end{aligned}
\tag{4.7}
$$

The real and imaginary parts of the polarization function can be seen in figure 4.1.

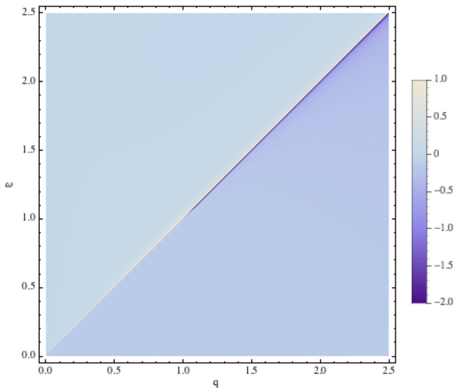

Figure 4.1.: Density plot of the real part of $P^{(1)}(q, \omega)$ in units of $\frac{\mu}{\hbar^2 v_F^2}$.

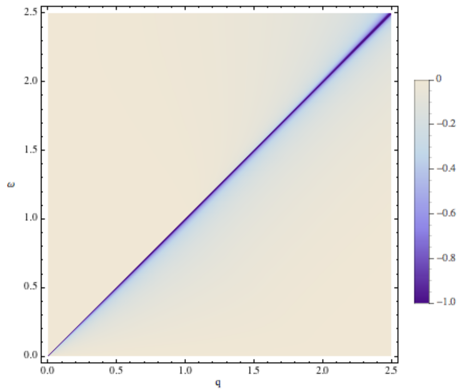

Figure 4.2.: Density plot of the imaginary part of $P^{(1)}(q, \omega)$ in units of $\frac{\mu}{\hbar^2 v_F^2}$.

In the self-consistent RPA the polarization is given by [13]:

Self-Consistent RPA Polarization

$$P_{RPA}(\vec{q}, \omega) = \frac{P^{(1)}(\vec{q}, \omega)}{1 - v_q P^{(1)}(\vec{q}, \omega)}, \tag{4.8}$$

where v_q denotes the in-plane Coulomb potential. Its real and imaginary part is plotted in fig 4.3 and 4.4.

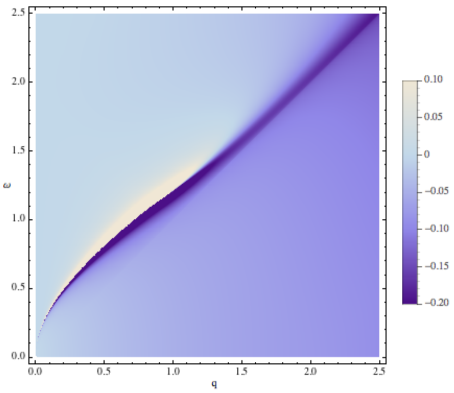

Figure 4.3.: Density plot of the real part of the renormalized polarization $P_{RPA}(\vec{q}, \omega)$ in units of $\frac{\mu}{\hbar^2 v_F^2}$.

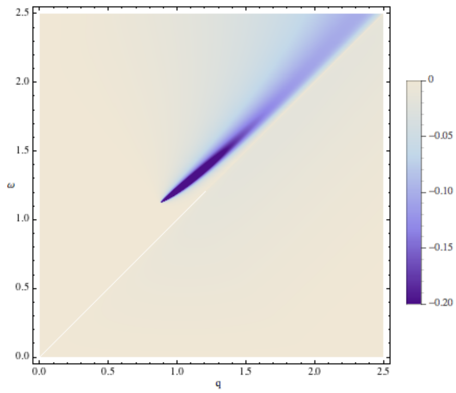

Figure 4.4.: Density plot of the imaginary part of the renormalized polarization $P_{RPA}(\vec{q}, \omega)$ in units of $\frac{\mu}{\hbar^2 v_F^2}$.

The existence of plasmons is reflected by the singularities that appear in the real part. Anyway, they are not yet what we are looking for, as this effect stems solely form the Dirac electrons themselves, without considering the new constituent equations for topological insulators.

4.2. 2D dielectric function and 2D conductivity

From the relation between the dielectric function and the polarization derived in (3.63) and the relation between the 2D conductance and the dielectric function found in (3.67), we get the last expressions needed to plot the dispersion relation of topological insulators.

The 2D dielectric function of 2D Dirac electron gas is given by

2D Dielectric Function of 2D Dirac Electron Gas

$$
\begin{aligned}
\epsilon(q,\omega)_{2D} = \epsilon_0 - \frac{e^2}{2q}\cdot\Bigg\{ & -\frac{g\mu}{2\pi\hbar^2 v_F^2} - \frac{igq^2}{16\hbar\sqrt{\omega^2 - q^2 v_F^2}} - \frac{gq^2}{16\pi\hbar\sqrt{\omega^2 - q^2 v_F^2}}\cdot \\
& \Bigg\{\Theta\left(\frac{2\mu-\omega\hbar}{q\hbar v_F} - 1\right)\cdot \\
& \left[\frac{(2\mu-\omega\hbar)\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - i\pi\ln\left(\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu-\omega\hbar}{q\hbar v_F}\right)\right] \\
& - \Theta\left(\frac{\omega\hbar-2\mu}{q\hbar v_F} + 1\right)\cdot \\
& \left[\frac{(\omega\hbar-2\mu)\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{\omega\hbar-2\mu}{q\hbar v_F}\right)\right] + \\
& + \left(\frac{(2\mu+\omega\hbar)\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu+\omega\hbar}{q\hbar v_F}\right)\right)\Bigg\}\Bigg\}
\end{aligned}
\tag{4.9}
$$

and the 2D conductivity by

2D conductivity of 2D Dirac Electron Gas

$$
\begin{aligned}
\bar{\sigma}_{2D} = i\frac{e^2}{q^2}\omega \cdot \Bigg\{ & -\frac{g\mu}{2\pi\hbar^2 v_F^2} - \frac{igq^2}{16\hbar\sqrt{\omega^2 - q^2 v_F^2}} - \frac{gq^2}{16\pi\hbar\sqrt{\omega^2 - q^2 v_F^2}} \cdot \\
& \Bigg\{ \Theta\left(\frac{2\mu - \omega\hbar}{q\hbar v_F} - 1\right) \cdot \\
& \left[\frac{(2\mu - \omega\hbar)\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - i\pi \ln\left(\sqrt{\frac{(2\mu - \omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu - \omega\hbar}{q\hbar v_F}\right)\right] \\
& - \Theta\left(\frac{\omega\hbar - 2\mu}{q\hbar v_F} + 1\right) \cdot \\
& \left[\frac{(\omega\hbar - 2\mu)\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(\omega\hbar - 2\mu)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{\omega\hbar - 2\mu}{q\hbar v_F}\right)\right] + \\
& + \left(\frac{(2\mu + \omega\hbar)\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(2\mu + \omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu + \omega\hbar}{q\hbar v_F}\right)\right)\Bigg\}\Bigg\}
\end{aligned}
\tag{4.10}
$$

4.3. Plasmon Dispersion Relation T.I.

We are now able to write down the final result of this thesis, the (implicit) plasmon dispersion relation of topological insulators by inserting (3.54) and (4.11) in (3.56), which we will not write down explicitly:

Plasmon Dispersion Relation of Topological Insulators

$$k_x^2 = \epsilon_i \mu_i \omega^2 - \Bigg(\frac{1}{2\pi^2 \left(\bar{\sigma}_{2D} k_2^z + \omega \epsilon_2\right)} \Big[\alpha^2 \Delta\theta^2 \omega \epsilon_0 k_2^z - \pi^2 \mu_0 \bar{\sigma}_{2D}^2 \omega k_2^z + \\ + \pi^2 \bar{\sigma}_{2D} (k_2^z)^2 + \pi^2 \omega \epsilon_1 k_2^z + \pi^2 \omega \epsilon_2 k_2^z - \pi^2 \mu_0 \bar{\sigma}_{2D} \omega^2 \epsilon_2 \\ - \left\{ \left(\omega k_2^z \left(\alpha^2 \Delta\theta^2 \epsilon_0 - \pi^2 \mu_0 \bar{\sigma}_{2D}^2 + \pi^2 \left(\epsilon_1 + \epsilon_2\right)\right) + \pi^2 \bar{\sigma}_{2D} (k_2^z)^2 - \pi^2 \mu_0 \bar{\sigma}_{2D} \omega^2 \epsilon_2 \right)^2 + \\ + 4\pi^4 \omega \epsilon_1 k_2^z \left(\mu_0 \bar{\sigma}_{2D} \omega - k_2^z\right) \left(\bar{\sigma}_{2D} k_2^z + \omega \epsilon_2\right) \right\}^{\frac{1}{2}} \Big] \Bigg)^2$$

with

$$\bar{\sigma}_{2D} = i \frac{e^2}{q^2} \omega \cdot \Bigg\{ - \frac{g\mu}{2\pi\hbar^2 v_F^2} - \frac{igq^2}{16\hbar\sqrt{\omega^2 - q^2 v_F^2}} - \frac{gq^2}{16\pi\hbar\sqrt{\omega^2 - q^2 v_F^2}} \cdot \\ \Bigg\{ \Theta\left(\frac{2\mu - \omega\hbar}{q\hbar v_F} - 1 \right) \cdot \\ \left[\frac{(2\mu - \omega\hbar)\sqrt{\frac{(2\mu-\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - i\pi \ln\left(\sqrt{\frac{(2\mu - \omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu - \omega\hbar}{q\hbar v_F} \right) \right] \\ - \Theta\left(\frac{\omega\hbar - 2\mu}{q\hbar v_F} + 1 \right) \cdot \\ \left[\frac{(\omega\hbar - 2\mu)\sqrt{\frac{(\omega\hbar-2\mu)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(\omega\hbar - 2\mu)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{\omega\hbar - 2\mu}{q\hbar v_F} \right) \right] + \\ + \left(\frac{(2\mu + \omega\hbar)\sqrt{\frac{(2\mu+\omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1}}{q\hbar v_F} - \ln\left(\sqrt{\frac{(2\mu + \omega\hbar)^2}{q^2\hbar^2 v_F^2} - 1} + \frac{2\mu + \omega\hbar}{q\hbar v_F} \right) \right) \Bigg\} \Bigg\}$$

and

$$k_2^z = - \sqrt{\frac{\omega^2}{\frac{c^2}{\frac{\epsilon_2}{\epsilon_0}}}} \tag{4.11}$$

Let us now examine this dispersion relation. Before varying parameters to get a better understanding of their impact and to maybe see more clearly how the dispersion relation looks like qualitatively, we start with realistic values, i.e. we set $\Delta\theta = \pi$, $\epsilon_{r2} = \frac{\epsilon_2}{\epsilon_0}$ equal 50, to describe the bulk behavior of a topologic insulator and take ϵ_{r1} to be 1, ergo vacuum. We hence find the following dispersion relation for a topological insulator surrounded by vacuum (resp. air):

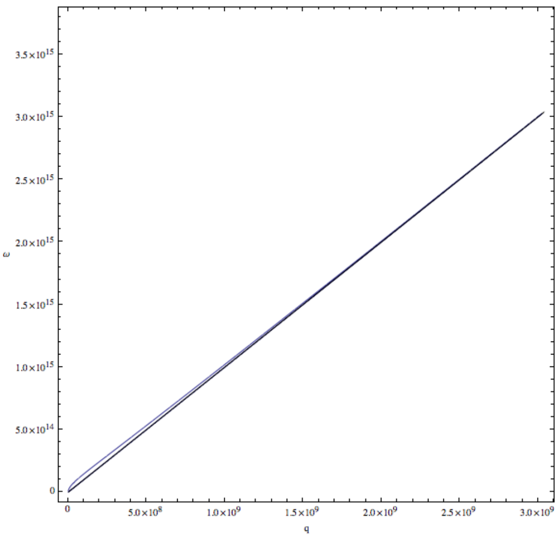

Figure 4.5.: Surface plasmon dispersion relation for a topological insulator with bulk dielectric constant $\epsilon_{r2} = 50$.

"Turning off" the the topological term by setting $\Delta\theta = 0$, we get

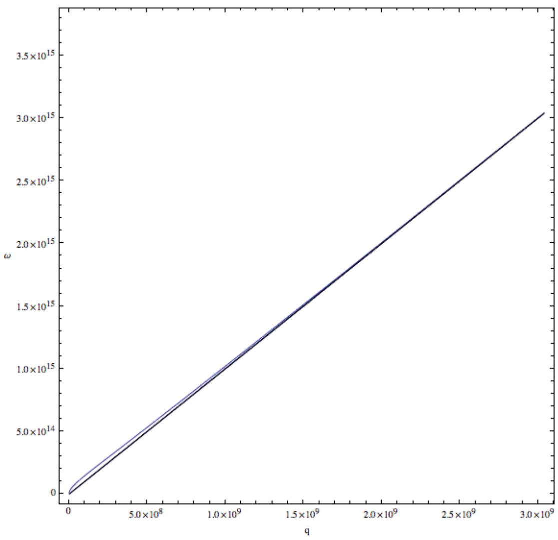

Figure 4.6.: Surface plasmon dispersion relation for a "topological insulator" with bulk dielectric constant $\epsilon_{r2} = 50$ setting $\Delta\theta = 0$.

what simply describes the dispersion relation of a gas of free massless Dirac electrons located between two dielectric media. Consequently, the effect of the topological term on plasmons for $\Delta\theta = \pi$ is hardly noticeable.

In a more detailed analysis of the topological electromagnetic effect than was done in 2.2.5, it can be seen, as mentioned, that the parameter $\Delta\theta$ can take any odd integer multiple of π, since it is related to the number of Dirac cones on the surface. We therefore plot the dispersion relation in this realistic model for different numbers of Dirac cones, i.e. different values for $\Delta\theta$.

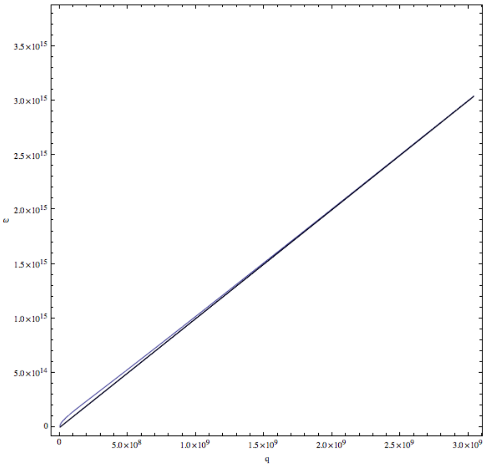

Figure 4.7.: Surface plasmon dispersion relation for $\epsilon_{r2} = 50$ and $\Delta\theta = 0$.

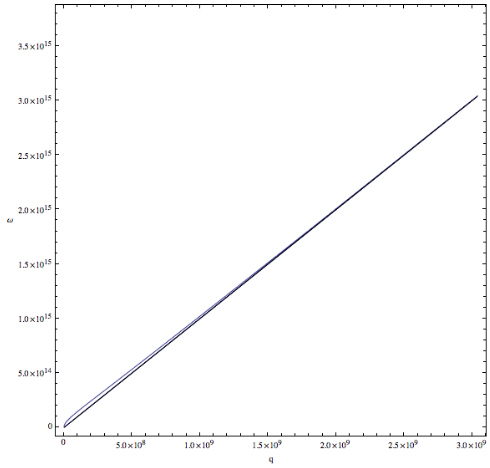

Figure 4.8.: Surface plasmon dispersion relation for $\epsilon_{r2} = 50$ and $\Delta\theta = 3\pi$.

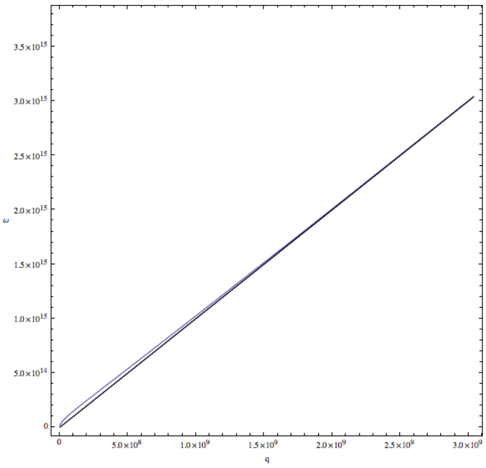

Figure 4.9.: Surface plasmon dispersion relation for $\epsilon_{r2} = 50$ and $\Delta\theta = 7\pi$.

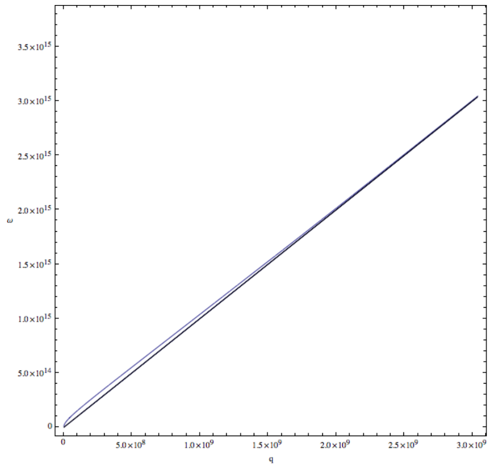

Figure 4.10.: Surface plasmon dispersion relation for $\epsilon_{r2} = 50$ and $\Delta\theta = 11\pi$.

To further examine the qualitative behavior of this relation, we decrease the value of ϵ_{r2} to 4 and resume our discussion as above:

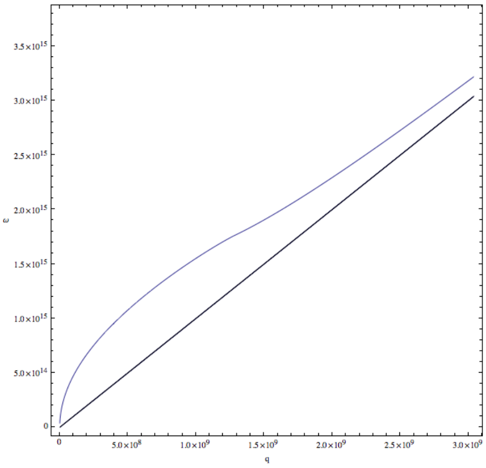

Figure 4.11.: Surface plasmon dispersion relation for $\epsilon_{r2} = 4$ and $\Delta\theta = 0$.

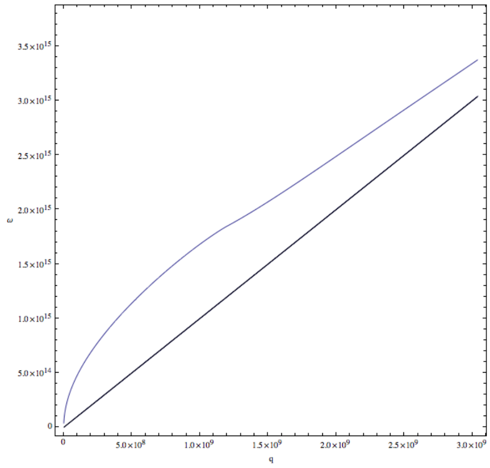

Figure 4.12.: Surface plasmon dispersion relation for $\epsilon_{r2} = 4$ and $\Delta\theta = \pi$.

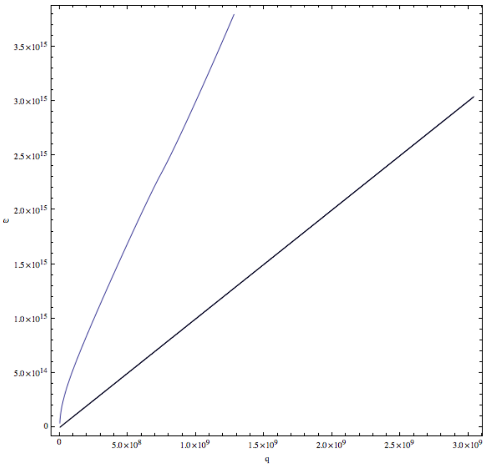

Figure 4.13.: Surface plasmon dispersion relation for $\epsilon_{r2} = 4$ and $\Delta\theta = 3\pi$.

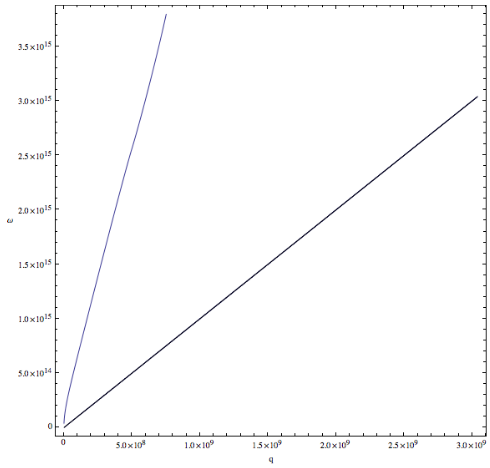

Figure 4.14.: Surface plasmon dispersion relation for $\epsilon_{r2} = 4$ and $\Delta\theta = 5\pi$.

The typical behavior of the free massless Dirac electron gas, as well as the effect of the varying parameter $\Delta\theta$ can here be seen much more clearly. Compared with the situation for $\Delta\theta = 0$, as seen in figure 4.11, including a topological term (figure 4.12, 4.13 and 4.14) changes the gradient of the dispersion relation what can be clearly seen and should be measurable in its quasi linear regime. As the gradient increases with the number of Dirac cones involved, detecting the plasmon dispersion relation also leads to the number of Dirac cones on the surface of the topological insulator. Anyway, significant effects are only present for small dielectric constants describing the bulk behavior of the topological insulator, or alternatively, a high number of Dirac cones on its surface.

5. Summary

We will here give a brief summery of what has been done and led us to our results. In a last figure we want to visualize again the qualitative behavior of the plasmon dispersion relation of topological insulators and its dependence on the number of Dirac cones.

5.1. What has been done

After shortly repeating the Maxwell equations, we introduced a new kind of material, known as topological insulator, a material, that is an insulator in its interior, but whose surface contains conducting states.
In order to classify and distinguish it from other phases of matter, we reviewed the concept of spontaneous symmetry breaking and presented topological order and symmetry protected topological order.
In the section about the topological magneto-electric effect, we sketched the derivation of new constitutive relations of topological insulators, before deriving the standard plasmon conditions and plasmon dispersion relation at an interface, giving the example of plasmons in a Drude gas.
As last part of our basic section we derived the polarization function in the random phase approximation based on the single particle Liouville-von-Neumann equation.

We then modeled surface plasmons in topological insulators by describing them as a two layer system, with one layer representing the bulk behavior of the topological insulator and the other layer being an arbitrary dielectric, or simply vacuum.
The conducting surface states were modeled by a surface charge density respectively

its conductance stemming from the free massless Dirac electrons.
Using the previously found constitutive relations of topological insulators, we derived new boundary conditions respectively a dispersion relation for plasmons in topological insulators.
After finding a general connection between the 2D conductivity and the 2D dielectric function, we calculated the permittivity of a gas of 2D free massless Dirac electrons.

We were then capable to give the final result of this thesis (4.11), the (implicit) plasmon dispersion relation of topological insulators. Its qualitative behavior in dependence on the number of Dirac cones is presented in figure 5.1.

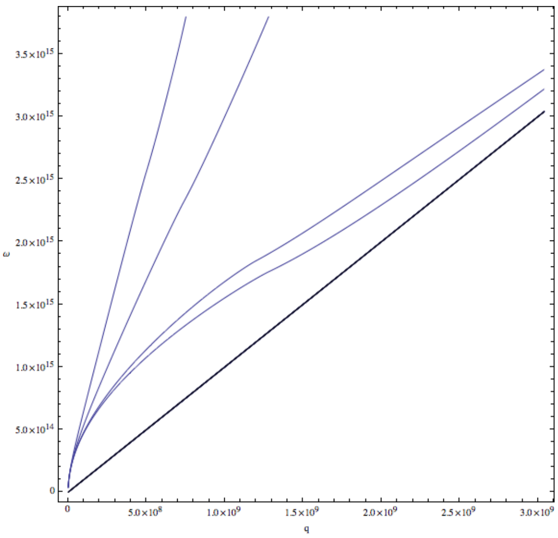

Figure 5.1.: Surface plasmon dispersion relations for a hypothetical topological insulator with bulk dielectric constant $\epsilon_{r2} = 4$ and various values for $\Delta\theta$. We start with $\Delta\theta = 0$. The dispersion relation gets steeper as we increase $\Delta\theta$ from π to 5π in steps of 2π.

5.2. Application and Outlook

Our formalism can be used to describe various plasmonic excitations on an interface. From the trivial case, with no charges, nor a topological term involved, to more sophisticated situations with a topological magneto electric effect on the boundary in the presence of several Dirac cones.
Significant effects are only present for small dielectric constants describing the bulk behavior of the topological insulator, limiting its applications significantly.
A slightly different use of our formalism can be found when describing monolayer structures on a substrate by describing the monolayer via its polarization function. Taking for example a monolayer of graphene on a substrate (e.g. SiO_2) yields results in line with literature.
Nevertheless, when dealing with a (hypothetical) topological insulator with lower dielectric constant, or alternatively, with a high number of Dirac cones on its surface, the results found in this work lead to experiments (and in consequence to devices) that could detect wether TR symmetry is broken in a topological insulator via a significant change in its plasmon dispersion relation, just like plasmonics is used nowadays to detect molecules.

Acknowledgments

I want to thank my supervisors Ulrich Hohenester and Christian Ertler for giving me the possibility to work on such an interesting subject of current interest and for their support throughout my thesis.
I really appreciate the great working environment I found here, with Ulrich Hohenester having an open door and ear for me all the time in his office next to mine and Christian Ertler always quickly answering to my mails even when being abroad. I am thankful for our regular meetings and discussions but also for being given the time to figure something out by my own.

I also want to express my gratitude to my colleagues and good friends Andreas Trügler and Jürgen Waxenegger for their inputs and identifying typos. A special thanks at this point again to Ulrich Hohenester, who not only supervised my work with regard to its content, but also took the time to check the orthography and made helpful remarks regarding phrasing - I do not take this for granted.

When doing research, there are times when you make big progress in very little time, but more often there is very little progress in big time. Anyway, when finding a working environment like I did, the challenge of finding solutions to problems (you might not even have thought of) becomes a great and enriching task and so I am happy to say that no matter how confusing the situation was sometimes: I enjoyed every single day.

A. Appendix – Utilities

A.1. Polarization Function of 2D free massless Dirac Fermions

$$\chi_D{}^{\beta}(\vec{q},\omega) = \frac{g}{4\pi^2\hbar}\int_{k\leq D}\sum_{\alpha=\pm}\frac{\alpha f^{\beta}(\vec{k},\vec{q})}{\omega+\alpha \mathrm{v}_F(k-\beta|\vec{k}+\vec{q}|)+\mathrm{i}0}d^2k \tag{A.1}$$

A.1.0.3. Imaginary Part

Using the identity

$$\frac{1}{x\pm \mathrm{i}0} = P\frac{1}{x}\mp i\pi\delta(x) \tag{A.2}$$

we get for the imaginary part :

$$-\frac{g}{4\pi}\int_0^{\tau} k\sum_{\alpha=\pm1}\alpha\int_0^{2\pi}\frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \\ \delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)d\theta dk \tag{A.3}$$

A.1.0.3.1. θ-Integration Calculation of the θ - integral :

$$k\int_0^{2\pi}\frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \\ \delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)d\theta \tag{A.4}$$

The only contribution we get from this integral is for

$$\delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)=1. \tag{A.5}$$

Therefore we have to find all zeros of

$$\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right) \tag{A.6}$$

regarding to θ.
We find (with the exceptions $\{\alpha=1,\beta=-1\}$, $\{\alpha=-1,\beta=1$ for $0<q<\omega$ and $\frac{1}{2}(-q+\omega)\leq k\leq\frac{q+\omega}{2}\}$, $\{\alpha=-1,\beta=-1,q>\omega$ and $k\geq\frac{q+\omega}{2}\}$)

$$\theta=-\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{A.7}$$

and

$$\theta=\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right) \tag{A.8}$$

As the arccos is only defined between (-1, 1)

$$1\geq\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\geq-1 \tag{A.9}$$

we get θ-functions of the form

$$\theta(\alpha)\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right) \tag{A.10}$$

for $\alpha=1$ and

$$\theta\left(-\alpha\right)\left(\theta\left(\omega-q\right)\left(\theta\left(\frac{\omega+q}{2}-k\right)-\theta\left(\frac{\omega-q}{2}-k\right)\right)+\right.$$
$$\left.\theta\left(q-\omega\right)\theta\left(k-\frac{q-\alpha\omega}{2}\right)\right) \tag{A.11}$$

for $\alpha = -1$.
This adds up to :

$$\theta(q-\omega)\theta\left(k - \frac{q-\alpha\omega}{2}\right) + \theta(-\alpha)\left(\theta(\omega - q)\left(\theta\left(\frac{\omega+q}{2} - k\right) - \theta\left(\frac{\omega-q}{2} - k\right)\right)\right) \quad \text{(A.12)}$$

With the substitution rule

$$\delta(g(x)) = \sum_{x_i : g(x_i)=0} \frac{\delta\left(x - x_i\right)}{\left|g'\left(x_i\right)\right|} \quad \text{(A.13)}$$

with the sum over all zeros of the δ - function we get :

$$\frac{d}{d\theta}\left(\omega + \alpha\left(k - \beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}\right)\right) = \frac{kq\alpha\beta\sin(\theta)}{\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \quad \text{(A.14)}$$

which leads to

$$-\frac{kq\alpha\beta\sqrt{1 - \frac{\left(q^2 - \omega(2k\alpha+\omega)\right)^2}{4k^2q^2}}}{\sqrt{k^2 + 2k\alpha\omega + \omega^2}} \quad \text{for}\theta = -\arccos\left(\frac{-q^2 + \omega(2k\alpha + \omega)}{2kq}\right) \quad \text{(A.15)}$$

and

$$\frac{kq\alpha\beta\sqrt{1 - \frac{\left(q^2 - \omega(2k\alpha+\omega)\right)^2}{4k^2q^2}}}{\sqrt{k^2 + 2k\alpha\omega + \omega^2}} \quad \text{for}\theta = \arccos\left(\frac{-q^2 + \omega(2k\alpha + \omega)}{2kq}\right) \quad \text{(A.16)}$$

The absolute value for both solutions is the same. The δ - function can now be written as

$$\delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)= \\ \left|\frac{\sqrt{k^2+2k\alpha\omega+\omega^2}}{kq\alpha\beta\sqrt{1-\frac{(q^2-\omega(2k\alpha+\omega))^2}{4k^2q^2}}}\right| \\ \left(\delta\left(\theta+\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right)\right)+\delta\left(\theta-\arccos\left(\frac{-q^2+\omega(2k\alpha+\omega)}{2kq}\right)\right)\right) \\ \left(\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right)\right. \\ \left.+\theta(-\alpha)\left(\theta(\omega-q)\left(\theta\left(\frac{\omega+q}{2}-k\right)-\theta\left(\frac{\omega-q}{2}-k\right)\right)\right)\right) \tag{A.17}$$

And the θ - integration yields :

$$\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta((q-\omega))\theta\left(k-\frac{q-\omega}{2}\right)+ \\ \sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right)+ \\ \sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right) \tag{A.18}$$

which is always real.

A.1.0.3.2. k-Integration Defining

$$I^{\alpha\beta}(k,q,\omega)=\sqrt{\frac{(2\alpha\mathrm{k}+\omega)^2-q^2}{(q^2-\omega^2)}}\left(\theta(\beta)\theta(q-\omega)\theta\left(k-\frac{q-\alpha\omega}{2}\right)+\right. \\ \left.\theta(-\beta)\theta(\omega-q)\theta(-\alpha)\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)\right), \tag{A.19}$$

for the k - integration we remember

$$
\begin{aligned}
&-\frac{g}{4\pi}\int_0^\tau k\sum_{\alpha=\pm 1}\alpha\int_0^{2\pi}\frac{1}{2}\left(1+\beta\frac{k+q*\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right)\\
&\delta\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)d\theta dk=\\
&-\frac{g}{4\pi}\int_0^\tau\sum_{\alpha=\pm 1}\alpha\mathrm{I}^{\alpha\beta}dk
\end{aligned}
\tag{A.20}
$$

For $\mu = 0$ (interband from cone underneath to upper cone - full band beneath, upper band empty) we get from the k - integration (Fermi function equal 1 in the cone beneath and zero in the upper cone)

$$
\begin{aligned}
&\mathrm{Im}P^0(\vec{q},\omega)=-\mathrm{Im}X_\Lambda{}^-(\vec{q},\omega)=\frac{g}{4\pi}\int_0^{\Lambda\to\infty}\sum_{\alpha=\pm 1}\alpha\mathrm{I}^{\alpha-}dk\\
&=-\frac{g}{4\pi}\int_0^\infty\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta(\omega-q)\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk\\
&=-\frac{gq^2\theta(-q+\omega)}{16\sqrt{-q^2+\omega^2}}
\end{aligned}
\tag{A.21}
$$

For $\mu > 0$ we get two additional contributions
(i) s = s' = 1 (intraband in the upper band)
(ii) interband contributions where the final state $E^{s'}(|\vec{k}+\vec{q}|) < \mu\,(n = n^0 + \delta\mathrm{n})$.

$$
\begin{aligned}
&\mathrm{Im}\Delta\mathrm{P}^1(\vec{q},\omega)=\mathrm{Im}\Delta\mathrm{P}^+(\vec{q},\omega)+\mathrm{Im}\Delta\mathrm{P}^-(\vec{q},\omega)=\\
&\mathrm{ImX}_{k_F}{}^+(q,\omega)+\mathrm{ImX}_{k_F}{}^-(q,\omega)=-\frac{g}{4\pi}\int_0^\mu\sum_{\alpha,\beta=\pm 1}\alpha\mathrm{I}^{\alpha\beta}dk=\\
&-\frac{g}{4\pi}\int_0^\mu\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk
\end{aligned}
\tag{A.22}
$$

Imaginary part in area 1A (0 < q < 2 μ, ω < q, ω < -q + 2 μ, ω > 0, q > 0, μ > 0)

$$
\begin{aligned}
&-\frac{g}{4\pi}\int_0^{\mu}\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk=
\end{aligned}
\tag{A.23}
$$

$$
\begin{aligned}
&=-\frac{g}{16\pi\sqrt{(q-\omega)(q+\omega)}}\Bigg((-2\mu+\omega)\sqrt{-q^2+(-2\mu+\omega)^2}\\
&+(2\mu+\omega)\sqrt{-q^2+(2\mu+\omega)^2}-q^2\ln\left(-\frac{-2\mu+\omega+\sqrt{-q^2+(-2\mu+\omega)^2}}{q}\right)\\
&+q^2\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\Bigg)
\end{aligned}
\tag{A.24}
$$

$$
\begin{aligned}
&=-\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\Bigg(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\\
&+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}-\ln\left(-\frac{-2\mu+\omega+\sqrt{-q^2+(-2\mu+\omega)^2}}{q}\right)\\
&+\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\Bigg)
\end{aligned}
\tag{A.25}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right.\\
&+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\\
&-\ln\left(\frac{\left(\frac{2\mu-\omega}{q}-\sqrt{-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)}{\left(\frac{2\mu-\omega}{q}+\sqrt{-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)}\left(\frac{2\mu-\omega}{q}+\sqrt{-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)\right)\\
&\left.-\ln\left(\frac{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}{q}\right)\right)
\end{aligned}
\tag{A.26}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right.\\
&+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}-\ln\left(\frac{\left(\left(\frac{2\mu-\omega}{q}\right)^2-\left(-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2\right)\right)}{\left(\frac{2\mu-\omega}{q}+\sqrt{-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)}\right)\\
&\left.-\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right)
\end{aligned}
\tag{A.27}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right.\\
&+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}+\ln\left(\frac{2\mu-\omega}{q}+\sqrt{-1^2+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)\\
&\left.-\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right)
\end{aligned}
\tag{A.28}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2} \right. \\
&\left. + \left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} + \operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right) - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right) \right)
\end{aligned} \tag{A.29}
$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2} \right. \\
&\left. -\operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right) - \left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} + \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right) \right)
\end{aligned} \tag{A.30}
$$

Imaginary part in area 2A ($\omega <$ q, $\omega >$ q - 2 μ, $\omega >$ -q + 2 μ, $\omega >$ 0, q > 0, $\mu >$ 0)

$$
\begin{aligned}
&- \frac{g}{4\pi}\int_0^{\mu} \sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right) \\
&- \sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right) \\
&- \sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right) - \theta\left(-k+\frac{-q+\omega}{2}\right)\right) dk = \\
&= -g\frac{(2\mu+\omega)\sqrt{-q^2+(2\mu+\omega)^2} + q^2\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)}{16\pi\sqrt{(q-\omega)(q+\omega)}}
\end{aligned} \tag{A.31}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \\
&\left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} + \ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right) \right.
\end{aligned} \tag{A.32}
$$

$$= -\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} - \ln\left(\frac{2\mu+\omega}{q} + \sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right) \tag{A.33}$$

Imaginary part in area 3A (q > 2 μ, $\omega <$ q - 2 μ, $\omega > 0$, q > 0, $\mu > 0$)

$$\begin{aligned} &-\frac{g}{4\pi}\int_0^\mu \sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right) \\ &-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right) \\ &-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q)) * \left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk = \\ &= 0 \end{aligned} \tag{A.34}$$

Imaginary part in area 1B (0 < q < μ, $\omega >$ q, $\omega <$ -q + 2 μ, $\omega > 0$, q > 0, $\mu > 0$)

$$\begin{aligned} &-\frac{g}{4\pi}\int_0^\mu \sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right) \\ &-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right) \\ &-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk = \\ &= \frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \end{aligned} \tag{A.35}$$

Imaginary part in area 2B (ω > q, ω < q + 2 μ, ω > -q + 2 μ, ω > 0, q > 0, μ > 0)

$$
\begin{aligned}
&-\frac{g}{4\pi}\int_0^{\mu}\sqrt{\frac{(2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q-\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{(q^2-\omega^2)}}\theta(q-\omega)\theta\left(k-\frac{q+\omega}{2}\right)\\
&-\sqrt{\frac{(-2k+\omega)^2-q^2}{q^2-\omega^2}}\theta((\omega-q))\left(\theta\left(-k+\frac{q+\omega}{2}\right)-\theta\left(-k+\frac{-q+\omega}{2}\right)\right)dk=
\end{aligned}
\tag{A.36}
$$

$$
\begin{aligned}
&=-\frac{g}{2}\left(2(2\mu-\omega)^3-q^2\left(4\mu-2\omega+\pi\sqrt{q^2-(-2\mu+\omega)^2}\right)\right.\\
&+iq^2\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}\left(2\ln\left(\frac{q}{\omega+\sqrt{-q^2+\omega^2}}\right)\right.\\
&+\ln\left(2i\mu-i\omega+\sqrt{q^2-(-2\mu+\omega)^2}\right)-\ln\left(-2i\mu+i\omega+\sqrt{q^2-(-2\mu+\omega)^2}\right)-\\
&\left.\left.\ln\left(-\frac{q^2+2\omega\left(-\omega+\sqrt{-q^2+\omega^2}\right)}{q^2}\right)\right)\right)\\
&\frac{1}{\left(16\pi\sqrt{-(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)}\right)}
\end{aligned}
\tag{A.37}
$$

Which can be simplified to

$$
=-\frac{g}{2}\frac{-\pi q^2+2(-2\mu+\omega)\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}-2q^2\arctan\left(\frac{2\mu-\omega}{\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}}\right)}{16\pi\sqrt{-q^2+\omega^2}}
\tag{A.38}
$$

$$
\begin{aligned}
&=-\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}}\frac{1}{q^2}\left(\frac{-\pi q^2}{2}+(-2\mu+\omega)\sqrt{(q+(2\mu-\omega))(q-(2\mu-\omega))}\right.\\
&\left.-q^2\arctan\left(\frac{2\mu-\omega}{\sqrt{(q+(2\mu-\omega))(q-(2\mu-\omega))}}\right)\right)
\end{aligned}
\tag{A.39}
$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} + \left(\frac{-2\mu+\omega}{q} \right) \sqrt{1 - \left(\frac{2\mu-\omega}{q} \right)^2} - \arctan\left(\frac{2\mu-\omega}{\sqrt{q^2-(2\mu-\omega)^2}} \right) \right) \tag{A.40}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q} \right) \sqrt{1 - \left(\frac{2\mu-\omega}{q} \right)^2} - \arctan\left(\frac{\frac{2\mu-\omega}{q}}{\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}} \right) \right) \tag{A.41}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q} \right) \sqrt{1 - \left(\frac{2\mu-\omega}{q} \right)^2} - \arctan\left(\frac{\frac{2\mu-\omega}{q}}{\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}} \right) \right) \tag{A.42}$$

for $\frac{2\mu-\omega}{q} > 0$:

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q} \right) \sqrt{1 - \left(\frac{2\mu-\omega}{q} \right)^2} - \arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}} \right) \right) \tag{A.43}$$

with

$$\arccos(x) = \frac{\pi}{2} - \operatorname{sign}(x) \arctan\sqrt{\frac{x^2}{1-x^2}} \tag{A.44}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arccos\left(\frac{2\mu-\omega}{q}\right) - \frac{\pi}{2}\right) \tag{A.45}$$

with

$$\arccos(-x) = \pi - \arccos(x) \tag{A.46}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(-\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(-\frac{2\mu-\omega}{q}\right)\right) \tag{A.47}$$

$$-\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\frac{-2\mu+\omega}{q}\right)\right) \tag{A.48}$$

for $\frac{2\mu-\omega}{q} < 0$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arctan\left(-\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right) \tag{A.49}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right) \tag{A.50}$$

with

$$\arccos(x) = \frac{\pi}{2} - \operatorname{sign}(x) \arctan \sqrt{\frac{x^2}{1-x^2}} \tag{A.51}$$

$$\begin{aligned} &= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \\ &\left(\frac{-\pi}{2} - \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arccos\left(\frac{2\mu-\omega}{q}\right) - \frac{\pi}{2} \right) \end{aligned} \tag{A.52}$$

with

$$\arccos(-x) = \pi - \arccos(x) \tag{A.53}$$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(-\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(-\frac{2\mu-\omega}{q}\right) \right) \tag{A.54}$$

$$-\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\frac{-2\mu+\omega}{q}\right) \right) \tag{A.55}$$

The solution is therefore independent of the sign of $\frac{2\mu-\omega}{q}$

$$= -\frac{gq^2}{16\pi\sqrt{-q^2+\omega^2}} \left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\frac{-2\mu+\omega}{q}\right) \right) \tag{A.56}$$

Imaginary part in area 3B ($\omega >$ q + 2 μ, $\omega > 0$, q > 0, $\mu > 0$) is 0.

A.1.0.4. Real Part

Lets now calculate the real part :

$$\int_0^\tau k * \int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)+\mathrm{i}0} d\theta dk \quad \text{(A.57)}$$

Using the identity

$$\frac{1}{x\pm \mathrm{i}0} = P\frac{1}{x} \mp i\pi\delta(x) \quad \text{(A.58)}$$

we get for the real part :

$$\frac{g}{4\pi^2}\int_0^\tau k \sum_{\alpha=\pm 1} \alpha \int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)} d\theta dk \quad \text{(A.59)}$$

A.1.0.4.1. θ-Integration Calculation of the θ - integral :

$$\alpha \int_0^{2\pi} \frac{1}{2}\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)} d\theta \quad \text{(A.60)}$$

The integrand can be simplified:

$$\left(1+\beta\frac{k+q\cos(\theta)}{\sqrt{k^2+q^2+2kq\cos(\theta)}}\right) \frac{1}{\left(\omega+\alpha\left(k-\beta\sqrt{k^2+q^2+2kq\cos(\theta)}\right)\right)} \quad \text{(A.61)}$$

$$= \left(\frac{\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)} + (k + q\cos(\theta))}{\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \right) \frac{\alpha}{(\omega + \alpha k) - \alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \tag{A.62}$$

$$= \left(\frac{\alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)} + \alpha(k + q\cos(\theta))}{\alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \right) \frac{\alpha}{(\omega + \alpha k) - \alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \tag{A.63}$$

Principal value integral at $x = 0$, thus $(\omega + \alpha k) = \alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}$

$$= \left(\frac{(\omega + \alpha k) + \alpha(k + q\cos(\theta))}{(\omega + \alpha k)} \right) \frac{\alpha}{(\omega + \alpha k) - \alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}} \tag{A.64}$$

$$= \alpha \left(\frac{(\omega + \alpha k) + \alpha(k + q\cos(\theta))}{(\omega + \alpha k)} \right) \frac{(\omega + \alpha k) + \alpha\beta\sqrt{k^2 + q^2 + 2kq\cos(\theta)}}{(\omega + \alpha k)^2 - (k^2 + q^2 + 2kq\cos(\theta))} \tag{A.65}$$

$$= \alpha \left(\frac{(\omega + \alpha k) + \alpha(k + q\cos(\theta))}{(\omega + \alpha k)} \right) \frac{(\omega + \alpha k) + (\omega + \alpha k)}{(\omega + \alpha k)^2 - (k^2 + q^2 + 2kq\cos(\theta))} \tag{A.66}$$

$$= 2\alpha(\omega + 2\alpha k + \alpha q\cos(\theta)) \frac{1}{(\omega + \alpha k)^2 - (k^2 + q^2 + 2kq\cos(\theta))} \tag{A.67}$$

$$2\frac{2k + \alpha\omega + q\cos(\theta)}{(k + \alpha\omega)^2 - (k^2 + q^2 + 2kq\cos(\theta))} \tag{A.68}$$

The θ - integral therefore reads:

$$\alpha \int_0^{2\pi} \frac{2k + \alpha\omega + q\cos(\theta)}{(k+\alpha\omega)^2 - (k^2 + q^2 + 2kq\cos(\theta))}\, d\theta \tag{A.69}$$

For $\alpha = 1$:

$$\alpha \int_0^{2\pi} \frac{2k + \omega + q\cos(\theta)}{(\omega+k)^2 - (k^2 + q^2 + 2kq\cos(\theta))}\, d\theta = \tag{A.70}$$

$$= \frac{\pi\left(2k\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}} + q\left(-1+\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right) + \omega\left(-1+\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}}\right)\right)}{k(q+\omega)} \tag{A.71}$$

For $(2k - q + \omega)(q + \omega) \neq 0\&\&(q - \omega)(2k + q + \omega) \neq 0$ and $\left(\mathrm{Re}\left(\frac{q^2-\omega(2k+\omega)}{kq}\right) \geq 2 \middle\| \mathrm{Re}\left(\frac{q^2-\omega(2k+\omega)}{kq}\right) \leq -2 \middle\| \frac{q^2-\omega(2k+\omega)}{kq} \notin \text{Reals}\right)$

$$= \frac{\pi\left(2k\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}} + q\left(-1+\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right) + \omega\left(-1+\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}}\right)\right)}{k(q+\omega)} \tag{A.72}$$

$$= \frac{\pi\left(2k\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}} + \left(-q+q\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right) + \left(-\omega+\omega\sqrt{\frac{(2k-q+\omega)(q+\omega)}{(-q+\omega)(2k+q+\omega)}}\right)\right)}{k(q+\omega)} \tag{A.73}$$

$$= \frac{\pi\left(2k\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}} + \left(-q+q\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right) + \left(-\omega+\omega\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right)\right)}{k(q+\omega)} \tag{A.74}$$

$$
\begin{aligned}
&= \frac{\pi\left((-q-\omega)+2k\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}+q\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}+\omega\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right)}{k(q+\omega)} \\
&= \frac{\pi\left((-q-\omega)+(2k+q+\omega)\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}\right)}{k(q+\omega)} \\
&= \frac{\pi(-q-\omega)}{k(q+\omega)}+\frac{\pi(2k+q+\omega)\sqrt{\frac{(-2k+q-\omega)(q+\omega)}{(q-\omega)(2k+q+\omega)}}}{k(q+\omega)} \\
&= -\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(-2k+q-\omega)(2k+q+\omega)(q+\omega)}{(q-\omega)}}}{k(q+\omega)} \\
&= -\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(-2k+q-\omega)(2k+q+\omega)}{(q+\omega)(q-\omega)}}}{k} \\
&= -\frac{\pi}{k}+\frac{\pi\sqrt{\frac{-(2k-q+\omega)(2k+q+\omega)}{q^2-\omega^2}}}{k} \\
&= -\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}
\end{aligned}
\tag{A.75}
$$

Looking at the conditional expression, we find

$$
\begin{aligned}
&(2k-q+\omega)(q+\omega)\neq 0\&\&(q-\omega)(2k+q+\omega)\neq 0\&\& \\
&\left(\mathrm{Re}\left(\frac{q^2-\omega(2k+\omega)}{kq}\right)\geq 2\middle\|\mathrm{Re}\left(\frac{q^2-\omega(2k+\omega)}{kq}\right)\leq -2\middle\|\frac{q^2-\omega(2k+\omega)}{kq}\notin \mathrm{Reals}\right)
\end{aligned}
\tag{A.76}
$$

$$
\begin{aligned}
\to\ &(2k-q+\omega)(q+\omega)\neq 0\&\&(q-\omega)(2k+q+\omega)\neq 0\&\& \\
&\left(\frac{q^2-\omega(2k+\omega)}{kq}\geq 2\|\frac{q^2-\omega(2k+\omega)}{kq}\leq -2\right)
\end{aligned}
\tag{A.77}
$$

$$\rightarrow (2k-q+\omega)(q+\omega)\neq 0\&\&(q-\omega)(2k+q+\omega)\neq 0\&\& \left(q^2-\omega(2k+\omega)\geq 2kq\|q^2-\omega(2k+\omega)\leq -2kq\right) \quad (A.78)$$

$$\rightarrow \omega > 0\&\&q > \omega\&\&0 < k < \frac{q-\omega}{2} \quad (A.79)$$

$$\rightarrow \theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right) \quad (A.80)$$

and

$$\rightarrow \omega > 0 \ \&\& \ 0 < \mathrm{q} < \omega \ \&\& \ \mathrm{k} > 0 \quad (A.81)$$

$$\rightarrow \theta(\omega-q) \quad (A.82)$$

Including the conditions we therefore get for $\alpha = 1$:

$$\left(-\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right) \quad (A.83)$$

For $\alpha = -1$:

$$\alpha\int_0^{2\pi}\frac{2k-\omega+q\cos(\theta)}{(\omega-k)^2-(k^2+q^2+2kq\cos(\theta))}\,d\theta = -\frac{\pi\left(2k+(q+\omega)\left(-1+\sqrt{\frac{(q-\omega)(-2k+q+\omega)}{(2k+q-\omega)(q+\omega)}}\right)\right)}{k(q+\omega)\sqrt{\frac{-2kq+q^2+2k\omega-\omega^2}{(2k+q-\omega)(q+\omega)}}} \quad (A.84)$$

For $(2k+q-\omega)(q+\omega)\neq 0\&\&q^2+2k\omega\neq 2kq+\omega^2$ and
$\left(\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\geq 2\left\|\left(\mathrm{Re}\left(\frac{-q^2+\omega(-2k+\omega)}{kq}\right)\geq 2\&\&\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\leq -2\right)\right\|\frac{q^2+2k\omega-\omega^2}{kq}\notin \mathrm{Reals}\right)$

This can further be simplified to

$$\begin{aligned}
&= \frac{\pi\left(-2k+q+\omega-\sqrt{\frac{(q-\omega)(q+\omega)(-2k+q+\omega)}{2k+q-\omega}}\right)}{k\sqrt{-\frac{(2k-q-\omega)(q-\omega)(q+\omega)}{2k+q-\omega}}} \\
&= \frac{\pi(-2k+q+\omega)}{k\sqrt{\frac{(-2k+q+\omega)(q-\omega)(q+\omega)}{2k+q-\omega}}} - \frac{\pi\sqrt{\frac{(q-\omega)(q+\omega)(-2k+q+\omega)}{2k+q-\omega}}}{k\sqrt{\frac{(-2k+q+\omega)(q-\omega)(q+\omega)}{2k+q-\omega}}} \\
&= -\frac{\pi}{k} + \frac{\pi(-2k+q+\omega)\sqrt{\frac{2k+q-\omega}{(-2k+q+\omega)(q-\omega)(q+\omega)}}}{k} \\
&\text{for q+}\omega\text{ >2k :} \\
&= -\frac{\pi}{k} + \frac{\pi\sqrt{\frac{(-2k+q+\omega)(2k+q-\omega)}{(q-\omega)(q+\omega)}}}{k} \\
&= -\frac{\pi}{k} + \frac{\pi\sqrt{\frac{-(2k-q-\omega)(2k+q-\omega)}{q^2-\omega^2}}}{k} \\
&= -\frac{\pi}{k} + \frac{\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}}{k} \\
&\text{for q+}\omega\text{ <2k:} \\
&= -\frac{\pi}{k} - \frac{\pi\sqrt{\frac{(-2k+q+\omega)(2k+q-\omega)}{(q-\omega)(q+\omega)}}}{k} \\
&= -\frac{\pi}{k} - \frac{\pi\sqrt{\frac{-(2k-q-\omega)(2k+q-\omega)}{q^2-\omega^2}}}{k} \\
&= -\frac{\pi}{k} - \frac{\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}
\end{aligned} \tag{A.85}$$

Looking at the conditional expression, we find

$$\begin{aligned}
&(2k+q-\omega)(q+\omega)\neq 0\&\&q^2+2k\omega\neq 2kq+\omega^2\&\& \\
&\quad\left(\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\geq 2\middle\|\left(\mathrm{Re}\left(\frac{-q^2+\omega(-2k+\omega)}{kq}\right)\geq 2\&\&\right.\right. \\
&\quad\quad\left.\left.\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\leq -2\right)\middle\|\frac{q^2+2k\omega-\omega^2}{kq}\notin \mathrm{Reals}\right)
\end{aligned} \tag{A.86}$$

$$\to (2k+q-\omega)(q+\omega)\neq 0\&\&q^2+2k\omega\neq 2kq+\omega^2\&\& \left(\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\geq 2\|\left(\mathrm{Re}\left(\frac{-q^2+\omega(-2k+\omega)}{kq}\right)\geq 2\&\&\mathrm{Re}\left(\frac{q^2+2k\omega-\omega^2}{kq}\right)\leq -2\right)\right) \tag{A.87}$$

$$\to (2k+q-\omega)(q+\omega)\neq 0\&\&q^2+2k\omega\neq 2kq+\omega^2\&\& \left(q^2+2k\omega-\omega^2\geq 2kq\|\left(-q^2+\omega(-2k+\omega)\geq 2kq\&\&q^2+2k\omega-\omega^2\leq -2kq\right)\right) \tag{A.88}$$

$$\to \omega>0\&\&\left(\left(0<q<\omega\&\&0<k<\frac{1}{2}(-q+\omega)\right)\|\left(q>\omega\&\&0<k<\frac{q+\omega}{2}\right)\right) \tag{A.89}$$

$$\to \theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right) \tag{A.90}$$

and

$$\to \omega>0\&\&0<q<\omega\&\&k>\frac{q+\omega}{2} \tag{A.91}$$

$$\to \theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right) \tag{A.92}$$

and the solution including the conditions reads

$$\left(-\frac{\pi}{k}+\frac{\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}\right) \left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)+ \left(-\frac{\pi}{k}-\frac{\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}}{k}\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right) \tag{A.93}$$

All together we get (where we already multiplied with k in the integrand)

$$\left(-\pi+\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)+ \\ \left(-\pi+\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right) \\ \left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)+ \\ \left(-\pi-\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right) \quad \text{(A.94)}$$

A.1.0.4.2. k-Integration For $\mu=0$ (interband from cone underneath to upper cone - full band beneath, upper band empty) we get using the Kramers - Kronig relation (Fermi function equal 1 in the cone beneath and zero in the upper cone)

$$\frac{1}{\pi}\int_{-\infty}^{\infty}d\omega'\left(-\frac{gq^2\theta(-q+\omega')}{16\sqrt{-q^2+\omega'^2}}\frac{1}{\omega'-\omega}\right) \\ =-\frac{gq^2\left(\arccos\left(-\frac{\omega}{q}\right)\right)}{16\pi\sqrt{q^2-\omega^2}}\theta(q-\omega) \quad \text{(A.95)}$$

For $\mu>0$ we get two additional contributions:
(i) s = s' = 1 (intraband in the upper band)
(ii) interband contributions where the final state $E^{s'}(|\vec{k}+\vec{q}|)<\mu\,(n=n^0+\delta\mathrm{n})$.
$-\pi$ is treated separately - it yields $-\frac{g\mu}{2\pi}$

$$\left(\pi\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)+ \\ \left(\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)+ \\ \left(-\pi\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right) \quad \text{(A.96)}$$

Real part in area 1A ($0 < q < 2\mu$, $\omega < q$, $\omega < -q + 2\mu$, $\omega > 0$, $q > 0$, $\mu > 0$)

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=-\frac{g\mu}{2\pi}
\end{aligned} \tag{A.97}$$

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=\frac{gq^2}{16\sqrt{q^2-\omega^2}}
\end{aligned} \tag{A.98}$$

Real part in area 2A ($\omega < q$, $\omega > q - 2\mu$, $\omega > -q + 2\mu$, $\omega > 0$, $q > 0$, $\mu > 0$)

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=-\frac{g\mu}{2\pi}
\end{aligned} \tag{A.99}$$

$$\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.$$
$$+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)$$
$$\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)\,dk$$
$$=\frac{g}{2\pi}\frac{\pi q^2+2(2\mu-\omega)\sqrt{q^2-(-2\mu+\omega)^2}+2q^2\arctan\left(\frac{2\mu-\omega}{\sqrt{q^2-(-2\mu+\omega)^2}}\right)}{16\sqrt{(q-\omega)(q+\omega)}}$$
$$=\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\frac{\pi}{2}+\left(\frac{2\mu-\omega}{q^2}\right)\sqrt{q^2-(-2\mu+\omega)^2}+\arctan\left(\frac{2\mu-\omega}{\sqrt{q^2-(-2\mu+\omega)^2}}\right)\right)$$
$$=\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\frac{\pi}{2}+\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}+\arctan\left(\frac{\frac{2\mu-\omega}{q}}{\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right) \tag{A.100}$$

for $\dfrac{2\mu-\omega}{q}>0:$

$$=\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\frac{\pi}{2}+\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}+\arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right)$$

with $\arccos(x)=\dfrac{\pi}{2}-\operatorname{sign}(x)\arctan\sqrt{\dfrac{x^2}{1-x^2}}$

$$=\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\frac{\pi}{2}+\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}-\arccos\left(\left(\frac{2\mu-\omega}{q}\right)\right)+\frac{\pi}{2}\right)$$
$$=\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}-\arccos\left(\left(\frac{2\mu-\omega}{q}\right)\right)+\pi\right) \tag{A.101}$$

$$\text{with } \arccos(-x) = \pi - \arccos(x):$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{2\mu-\omega}{q}\right) \sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arccos\left(\left(-\frac{2\mu-\omega}{q}\right)\right)\right) \tag{A.102}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(-\left(\frac{\omega-2\mu}{q}\right) \sqrt{1-\left(\frac{\omega-2\mu}{q}\right)^2} + \arccos\left(\left(\frac{\omega-2\mu}{q}\right)\right)\right)$$

for $\frac{2\mu-\omega}{q} < 0$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\frac{\pi}{2} + \left(\frac{2\mu-\omega}{q}\right) \sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arctan\left(-\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right)$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\frac{\pi}{2} + \left(\frac{2\mu-\omega}{q}\right) \sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right) \tag{A.103}$$

$$
\begin{aligned}
&\text{with } \arccos(x) = \frac{\pi}{2} - \operatorname{sign}(x) \arctan\sqrt{\frac{x^2}{1-x^2}} \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\frac{\pi}{2} + \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)\right) \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\frac{\pi}{2} + \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \left(\arccos\left(\left(\frac{2\mu-\omega}{q}\right)\right) - \frac{\pi}{2}\right)\right) \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\frac{\pi}{2} + \left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\left(\frac{2\mu-\omega}{q}\right)\right) + \frac{\pi}{2}\right) \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} - \arccos\left(\left(\frac{2\mu-\omega}{q}\right)\right) + \pi\right) \\
&\text{with } \arccos(-x) = \pi - \arccos(x): \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arccos\left(\left(-\frac{2\mu-\omega}{q}\right)\right)\right) \\
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(-\left(\frac{\omega-2\mu}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \arccos\left(\left(\frac{\omega-2\mu}{q}\right)\right)\right)
\end{aligned}
\tag{A.104}
$$

The solution is therefore independent of the sign of $\frac{2\mu-\omega}{q}$

$$
\frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(-\left(\frac{\omega-2\mu}{q}\right)\sqrt{1-\left(\frac{\omega-2\mu}{q}\right)^2} + \arccos\left(\left(\frac{\omega-2\mu}{q}\right)\right)\right), \qquad \operatorname{Abs}\left(\frac{\omega-2\mu}{q}\right) < 1 \tag{A.105}
$$

Real part in area 3A (q > 2 μ, ω < q - 2 μ, $\omega > 0$, q > 0, $\mu > 0$)

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)\,dk\\
&=-\frac{g\mu}{2\pi}
\end{aligned}\tag{A.106}$$

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)\,dk\\
&=\frac{g}{2\pi}\frac{1}{16\sqrt{(q-\omega)(q+\omega)\left(q^4+\left(-4\mu^2+\omega^2\right)^2-2q^2\left(4\mu^2+\omega^2\right)\right)}}\\
&\left(2\left(-8\mu^3\sqrt{q^2-(-2\mu+\omega)^2}-12\mu^2\omega\sqrt{q^2-(-2\mu+\omega)^2}-6\mu\omega^2\sqrt{q^2-(-2\mu+\omega)^2}\right.\right.\\
&-\omega^3\sqrt{q^2-(-2\mu+\omega)^2}-8\mu^3\sqrt{q^2-(2\mu+\omega)^2}+12\mu^2\omega\sqrt{q^2-(2\mu+\omega)^2}\\
&-6\mu\omega^2\sqrt{q^2-(2\mu+\omega)^2}+\omega^3\sqrt{q^2-(2\mu+\omega)^2}\\
&+q^2\left(\omega\left(\sqrt{q^2-(-2\mu+\omega)^2}-\sqrt{q^2-(2\mu+\omega)^2}\right)\right.\\
&\left.\left.+2\mu\left(\sqrt{q^2-(-2\mu+\omega)^2}+\sqrt{q^2-(2\mu+\omega)^2}\right)\right)\right)\\
&+q^2\sqrt{q^4+\left(-4\mu^2+\omega^2\right)^2-2q^2\left(4\mu^2+\omega^2\right)}\left(2\arctan\left(\frac{2\mu+\omega}{\sqrt{q^2-(2\mu+\omega)^2}}\right)\right.\\
&\left.\left.-i\left(\ln\left(2i\mu-i\omega+\sqrt{q^2-(-2\mu+\omega)^2}\right)-\ln\left(-2i\mu+i\omega+\sqrt{q^2-(-2\mu+\omega)^2}\right)\right)\right)\right)
\end{aligned}\tag{A.107}$$

which can be simplified further to

$$= \frac{g}{16\pi\sqrt{(q-\omega)(q+\omega)}}$$
$$\Bigg(\omega\left(-\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}+\sqrt{(q-2\mu-\omega)(q+2\mu+\omega)}\right)$$
$$+\,2\mu\left(\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}+\sqrt{(q-2\mu-\omega)(q+2\mu+\omega)}\right)$$
$$+q^2\left(\arctan\left(\frac{2\mu-\omega}{\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}}\right)+\arctan\left(\frac{2\mu+\omega}{\sqrt{q^2-(2\mu+\omega)^2}}\right)\right)\Bigg) \tag{A.108}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\frac{1}{q^2}\Bigg(\omega\left(-\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}+\sqrt{(q-2\mu-\omega)(q+2\mu+\omega)}\right)$$
$$+\,2\mu\left(\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}+\sqrt{(q-2\mu-\omega)(q+2\mu+\omega)}\right)$$
$$+q^2\left(\arctan\left(\frac{2\mu-\omega}{\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}}\right)+\arctan\left(\frac{2\mu+\omega}{\sqrt{q^2-(2\mu+\omega)^2}}\right)\right)\Bigg) \tag{A.109}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\frac{1}{q^2}\Bigg(\left((2\mu-\omega)\sqrt{(q+2\mu-\omega)(q-2\mu+\omega)}+(2\mu+\omega)\sqrt{(q-2\mu-\omega)(q+2\mu+\omega)}\right)$$
$$+q^2\left(\arctan\left(\frac{2\mu-\omega}{\sqrt{q^2-(2\mu-\omega)^2}}\right)+\arctan\left(\frac{2\mu+\omega}{\sqrt{q^2-(2\mu+\omega)^2}}\right)\right)\Bigg) \tag{A.110}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\left(\left(\left(\frac{2\mu-\omega}{q^2}\right)\sqrt{q^2-(2\mu-\omega)^2}+\left(\frac{2\mu+\omega}{q^2}\right)\sqrt{q^2-(2\mu+\omega)^2}\right)\right. \tag{A.111}$$
$$\left.+\left(\arctan\left(\frac{2\mu-\omega}{\sqrt{q^2-(2\mu-\omega)^2}}\right)+\arctan\left(\frac{2\mu+\omega}{\sqrt{q^2-(2\mu+\omega)^2}}\right)\right)\right)$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right. \tag{A.112}$$
$$\left.+\left(\arctan\left(\frac{\frac{2\mu-\omega}{q}}{\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)+\arctan\left(\frac{\frac{2\mu+\omega}{q}}{\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}}\right)\right)\right)$$

for $\frac{2\mu-\omega}{q} > 0$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}}$$
$$\left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right. \tag{A.113}$$
$$\left.+\left(\arctan\left(\sqrt{\frac{\left(\frac{2\mu-\omega}{q}\right)^2}{1-\left(\frac{2\mu-\omega}{q}\right)^2}}\right)+\arctan\left(\sqrt{\frac{\left(\frac{2\mu+\omega}{q}\right)^2}{1-\left(\frac{2\mu+\omega}{q}\right)^2}}\right)\right)\right)$$

with $\arccos(x) = \frac{\pi}{2} - \mathrm{sign}(x)\arctan\sqrt{\frac{x^2}{1-x^2}}$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right) + \left(-\arccos\left(\frac{2\mu-\omega}{q}\right) + \frac{\pi}{2} - \arccos\left(\frac{2\mu+\omega}{q}\right) + \frac{\pi}{2}\right)\right) \tag{A.114}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right) + \left(-\arccos\left(\frac{2\mu-\omega}{q}\right) + \pi - \arccos\left(\frac{2\mu+\omega}{q}\right)\right)\right) \tag{A.115}$$

with

$$\arccos(-x) = \pi - \arccos(x) \tag{A.116}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right) + \left(\arccos\left(-\frac{2\mu-\omega}{q}\right) - \arccos\left(\frac{2\mu+\omega}{q}\right)\right)\right) \tag{A.117}$$

$$= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \left(\left(\left(\frac{2\mu-\omega}{q}\right)\sqrt{1-\left(\frac{2\mu-\omega}{q}\right)^2} + \left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}\right) + \left(\arccos\left(\frac{\omega-2\mu}{q}\right) - \arccos\left(\frac{2\mu+\omega}{q}\right)\right)\right) \tag{A.118}$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{q^2-\omega^2}} \\
&\left(\left(-\left(\frac{\omega-2\mu}{q}\right)\sqrt{1-\left(\frac{\omega-2\mu}{q}\right)^2}+\arccos\left(\frac{\omega-2\mu}{q}\right)\right)\right. \\
&\left.+\left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{1-\left(\frac{2\mu+\omega}{q}\right)^2}-\arccos\left(\frac{2\mu+\omega}{q}\right)\right)\right)
\end{aligned}
\tag{A.119}
$$

for $\left|\frac{\omega-2\mu}{q}\right| < 1$.

Real part in area 1B (0 < q < μ, ω > q, ω < -q + 2 μ, ω > 0, q > 0, μ > 0)

$$
\begin{aligned}
&\frac{g}{4\pi}\int_0^\mu \left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right. \\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right) \\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)\,dk \\
&= -\frac{g\mu}{2\pi}
\end{aligned}
\tag{A.120}
$$

$$\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.$$
$$+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)$$
$$\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)\,dk$$
$$=-\frac{g}{16\pi(q-\omega)(q+\omega)}\sqrt{-q^2+\omega^2}$$
$$\left(-2\mu\sqrt{-q^2+(-2\mu+\omega)^2}+\omega\sqrt{-q^2+(-2\mu+\omega)^2}+2\mu\sqrt{-q^2+(2\mu+\omega)^2}\right.$$
$$+\omega\sqrt{-q^2+(2\mu+\omega)^2}+q^2\ln(q)+q^2\ln\left(\frac{q}{\omega+\sqrt{-q^2+\omega^2}}\right)+q^2\ln\left(\omega+\sqrt{-q^2+\omega^2}\right)$$
$$\left.-q^2\ln\left(2\mu-\omega-\sqrt{-q^2+(-2\mu+\omega)^2}\right)-q^2\ln\left(2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}\right)\right) \tag{A.121}$$

$$=\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}}$$
$$\frac{1}{q^2}\left((-2\mu+\omega)\sqrt{-q^2+(-2\mu+\omega)^2}+(2\mu+\omega)\sqrt{-q^2+(2\mu+\omega)^2}+q^2\ln(q)+q^2\ln(q)\right.$$
$$\left.-q^2\ln\left(2\mu-\omega-\sqrt{-q^2+(-2\mu+\omega)^2}\right)-q^2\ln\left(2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}\right)\right) \tag{A.122}$$

$$=\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}}$$
$$\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right.$$
$$\left.+\ln\left(\frac{q}{2\mu-\omega-\sqrt{-q^2+(-2\mu+\omega)^2}}\right)+\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\right) \tag{A.123}$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\ln\left(\frac{1}{\frac{2\mu-\omega}{q}-\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}}\right)+\ln\left(\frac{1}{\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}}\right)\right)
\end{aligned} \tag{A.124}
$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&+\ln\left(\frac{\frac{2\mu-\omega}{q}+\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}}{\left(\frac{2\mu-\omega}{q}-\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)\left(\frac{2\mu-\omega}{q}+\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)}\right) \\
&-\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right.
\end{aligned} \tag{A.125}
$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\ln\left(\frac{\frac{2\mu-\omega}{q}+\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}}{\left(\left(\frac{2\mu-\omega}{q}\right)^2-\left(-1+\left(\frac{-2\mu+\omega}{q}\right)^2\right)\right)}\right)-\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right)
\end{aligned} \tag{A.126}
$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\ln\left(\frac{2\mu-\omega}{q}+\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}\right)-\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right)
\end{aligned} \tag{A.127}
$$

with $\operatorname{arccosh}(x) = \ln\left(x+\sqrt{x^2-1}\right)$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{-2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{-2\mu+\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right)-\operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right)
\end{aligned} \tag{A.128}
$$

$$
\begin{aligned}
&= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(-\left(\frac{2\mu-\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right)-\operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right)
\end{aligned} \tag{A.129}
$$

$$
\begin{aligned}
= \frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} &\left(-\left(\frac{2\mu-\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}+\operatorname{arccosh}\left(\frac{2\mu-\omega}{q}\right)\right. \\
&\left.+\left(\frac{2\mu+\omega}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}-\operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right)
\end{aligned} \tag{A.130}
$$

Real part in area 2B (ω > q, ω < q + 2 μ, ω > -q + 2 μ, ω > 0, q > 0, μ > 0)

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=-\frac{g\mu}{2\pi}
\end{aligned} \tag{A.131}$$

$$\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=\frac{g}{2\pi}\frac{(2\mu+\omega)\left(-q^2+(2\mu+\omega)^2\right)+q^2\sqrt{-q^2+(2\mu+\omega)^2}\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)}{8\sqrt{(q-\omega)(q+\omega)\left(q^2-(2\mu+\omega)^2\right)}}
\end{aligned} \tag{A.132}$$

$$=g\frac{(2\mu+\omega)\left(-q^2+(2\mu+\omega)^2\right)+q^2\sqrt{-q^2+(2\mu+\omega)^2}\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)}{16\pi\sqrt{(-q+\omega)(q+\omega)\left(-q^2+(2\mu+\omega)^2\right)}} \tag{A.133}$$

$$\begin{aligned}
&=\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}}\\
&\frac{\frac{1}{q^2}\left((2\mu+\omega)\left(-q^2+(2\mu+\omega)^2\right)+q^2\sqrt{-q^2+(2\mu+\omega)^2}\ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\right)}{\sqrt{\left(-q^2+(2\mu+\omega)^2\right)}}
\end{aligned} \tag{A.134}$$

$$= \frac{gq^2}{16\pi\sqrt{\omega^2 - q^2}} \frac{1}{q^2}\left((2\mu+\omega)\sqrt{(-q^2+(2\mu+\omega)^2)} + q^2 \ \ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\right) \tag{A.135}$$

$$= \frac{gq^2}{16\pi\sqrt{\omega^2 - q^2}} \left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{\left(-1+\left(\frac{2\mu+\omega}{q}\right)^2\right)} + \ \ln\left(\frac{q}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\right) \tag{A.136}$$

$$= \frac{gq^2}{16\pi\sqrt{\omega^2 - q^2}} \left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{\left(-1+\left(\frac{2\mu+\omega}{q}\right)^2\right)} + \ \ln\left(\frac{1}{\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}}\right)\right) \tag{A.137}$$

$$= \frac{gq^2}{16\pi\sqrt{\omega^2 - q^2}} \left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{\left(-1+\left(\frac{2\mu+\omega}{q}\right)^2\right)} - \ \ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right)\right) \tag{A.138}$$

$$= \frac{gq^2}{16\pi\sqrt{\omega^2 - q^2}} \left(\left(\frac{2\mu+\omega}{q}\right)\sqrt{\left(-1+\left(\frac{2\mu+\omega}{q}\right)^2\right)} - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right) \tag{A.139}$$

Real part in area 3B (ω > q + 2 μ, ω > 0, q > 0, μ > 0)

$$
\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left((-1)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+(-1)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+(-1)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=-\frac{g\mu}{2\pi}
\end{aligned}
\tag{A.140}
$$

$$
\begin{aligned}
&\frac{g}{4\pi}\int_0^{\mu}\left(\left(\sqrt{\frac{(2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(q-\omega)\theta\left(\frac{q-\omega}{2}-k\right)+\theta(\omega-q)\right)\right.\\
&+\left(\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\left(\theta(\omega-q)\theta\left(\frac{-q+\omega}{2}-k\right)+\theta(q-\omega)\theta\left(\frac{q+\omega}{2}-k\right)\right)\\
&\left.+\left(-\sqrt{\frac{(-2k+\omega)^2-q^2}{\omega^2-q^2}}\right)\theta(\omega-q)\theta\left(k-\frac{q+\omega}{2}\right)\right)dk\\
&=\frac{g}{4\pi^2}\left(\left(\pi\left((2\mu-\omega)^3+q^2(-2\mu+\omega)+\omega\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)}\right.\right.\right.\\
&+q^2\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}\left(-\ln\left(\omega+\sqrt{-q^2+\omega^2}\right)\right.\\
&\left.\left.\left.\left.+\ln\left(-2\mu+\omega+\sqrt{-q^2+(-2\mu+\omega)^2}\right)\right)\right)\right)\frac{1}{\left(4\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)}\right)}\\
&+\left(\pi\left(-q^2(2\mu+\omega)+(2\mu+\omega)^3-\omega\sqrt{(q-\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}+\right.\right.\\
&\left.\left.q^2\sqrt{-q^2+(2\mu+\omega)^2}\ln\left(\frac{\omega+\sqrt{-q^2+\omega^2}}{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}\right)\right)\right)\\
&\left.\frac{1}{\left(4\sqrt{(q-\omega)(q+\omega)\left(q^2-(2\mu+\omega)^2\right)}\right)}\right)
\end{aligned}
\tag{A.141}
$$

which can be simplified further to

$$
\begin{aligned}
&= \frac{g}{16\pi(q-\omega)(q+\omega)} \\
&\Bigg(\omega\Bigg(\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&-\sqrt{(q-\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&-2\mu\Bigg(\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&+\sqrt{(q-\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&+q^2\sqrt{-q^2+\omega^2}\ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)\Bigg)
\end{aligned} \tag{A.142}
$$

$$
\begin{aligned}
&= \frac{g}{16\pi(q-\omega)(q+\omega)} \\
&\Bigg(\omega\Bigg(\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&-\sqrt{(q-\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&-2\mu\Bigg(\sqrt{(q-\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&+\sqrt{(q-\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&+q^2\sqrt{-q^2+\omega^2}\ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)\Bigg)
\end{aligned} \tag{A.143}
$$

$$
\begin{aligned}
&= -\frac{g}{16\pi(-q+\omega)(q+\omega)} \\
&\Bigg(\omega\Bigg(\sqrt{-(-q+\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&-\sqrt{-(-q+\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&-2\mu\Bigg(\sqrt{-(-q+\omega)(q+2\mu-\omega)(q+\omega)(q-2\mu+\omega)} \\
&+\sqrt{-(-q+\omega)(q-2\mu-\omega)(q+\omega)(q+2\mu+\omega)}\Bigg) \\
&+q^2\sqrt{-q^2+\omega^2}\ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)\Bigg)
\end{aligned}
\tag{A.144}
$$

$$
\begin{aligned}
&-\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\frac{1}{q^2}\Bigg(\omega\left(\sqrt{-(q+2\mu-\omega)\ (q-2\mu+\omega)}-\sqrt{-(q-2\mu-\omega)\ (q+2\mu+\omega)}\right) \\
&-2\mu\left(\sqrt{-(q+2\mu-\omega)\ (q-2\mu+\omega)}+\sqrt{-(q-2\mu-\omega)(q+2\mu+\omega)}\right) \\
&+q^2\ \ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)\Bigg)
\end{aligned}
\tag{A.145}
$$

$$
\begin{aligned}
&-\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\frac{1}{q^2}\Bigg((\omega-2\mu)\sqrt{-(q+2\mu-\omega)\ (q-2\mu+\omega)}-(\omega+2\mu)\sqrt{-(q-2\mu-\omega)\ (q+2\mu+\omega)} \\
&+q^2\ \ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)\Bigg)
\end{aligned}
\tag{A.146}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\frac{1}{q^2}\Bigg((\omega-2\mu)\sqrt{-q^2+(2\mu-\omega)^2}-(\omega+2\mu)\sqrt{-q^2+(2\mu+\omega)^2} \\
&+q^2\ \ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}\right)+q^2\ \ln(q)-q^2\ \ln(q)\Bigg)
\end{aligned}
\tag{A.147}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}-\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&+\ \ln\left(2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}\right) \\
&\left.-\ln\left(-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}\right)+\ \ln(q)-\ \ln(q)\right)
\end{aligned}
\tag{A.148}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}-\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&+\ \ln\left(\frac{2\mu+\omega+\sqrt{-q^2+4\mu^2+4\mu\omega+\omega^2}}{q}\right) \\
&\left.-\ln\left(\frac{-2\mu+\omega+\sqrt{-(q+2\mu-\omega)(q-2\mu+\omega)}}{q}\right)\right)
\end{aligned}
\tag{A.149}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}-\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&+\ \ln\left(\frac{2\mu+\omega+\sqrt{-q^2+(2\mu+\omega)^2}}{q}\right) \\
&\left.-\ln\left(\frac{-2\mu+\omega+\sqrt{-q^2+(2\mu-\omega)^2}}{q}\right)\right)
\end{aligned} \tag{A.150}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}-\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&+\ln\left(\frac{2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right) \\
&\left.-\ln\left(\frac{-2\mu+\omega}{q}+\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}\right)\right)
\end{aligned} \tag{A.151}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu-\omega}{q}\right)^2}-\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2}\right. \\
&\left.+\ \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)-\operatorname{arccosh}\left(\frac{-2\mu+\omega}{q}\right)\right)
\end{aligned} \tag{A.152}
$$

$$
\begin{aligned}
&= -\frac{gq^2}{16\pi\sqrt{\omega^2-q^2}} \\
&\left(\left(\left(\frac{\omega-2\mu}{q}\right)\sqrt{-1+\left(\frac{\omega-2\mu}{q}\right)^2} - \operatorname{arccosh}\left(\frac{\omega-2\mu}{q}\right)\right)\right. \\
&\left. - \left(\left(\frac{\omega+2\mu}{q}\right)\sqrt{-1+\left(\frac{2\mu+\omega}{q}\right)^2} - \operatorname{arccosh}\left(\frac{2\mu+\omega}{q}\right)\right)\right)
\end{aligned}
\tag{A.153}
$$

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