The role of pseudospin in the optical and electronic properties of relativistic materials

by

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ABSTRACT

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This thesis focuses on the theoretical analysis of response functions, namely the optical conductivity and the dielectric function, of relativistic materials described by various values of pseudospin. Graphene, first theorized in 1947 but only discovered in 2004, is the hallmark two-dimensional relativistic material. The dynamics of low-energy quasiparticle excitations in graphene are described by the relativistic Dirac equation, despite the lack of any motion occurring at relativistic speeds. In addition to carrying the intrinsic spin of the electron, the Dirac fermions in graphene are imbued with an additional quantum spin-1/2 angular momentum referred to as pseudospin. Extending the mathematical theory behind graphene, it is possible to consider materials with pseudospin values higher than 1/2. The promise of graphene in future technologies and the remarkable behaviour in its quasiparticles prompts the search for other relativistic materials. Response functions are useful in this endeavour in that they describe the way that a specific system will interact with an experimental probe, allowing for the identification of new materials. These functions also carry a large amount of information about the system under study, more than can be surmised from the band structure alone. In this thesis, the magneto-optical conductivity of higher-pseudospin two-dimensional Dirac materials is analyzed. Signatures unique to each system are identified with the help of snowshoe diagrams. The same analysis is performed on the Kane system, a 3D model describing small-gap zincblende semiconductors. Under certain approximations, the Kane model exhibits massless excitations which are shown to be hybrid pseudospin-1/2 and pseudospin-1 Dirac fermions. This is then applied to a particular phase of the zincblende material HgCdTe in order to calculate its optical absorbance spectra and compare with experiment. Finally, the pseudospin-1 system is focused on specifically through the
full derivation of the dynamical polarizability. This function describes all of the dielectric properties of the material, which in turn renormalizes the Coulomb interaction between charged species. The pseudospin-1 polarizability is compared to that of the pseudospin-1/2 system, showing novel differences due to the presence of a flat band fixed at zero energy in the former system. From the dielectric function, some of the collective behaviour of the pseudospin-1 system is analyzed (plasmon excitations and screening around electromagnetic impurities).
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Chapter 1

Motivation

The discovery of graphene by Novoselov and Geim in 2004 [1], along with subsequent investigations [2,3], created a boom in the study of relativistic condensed matter systems. The material was first discussed as a stand-alone system by Canadian theoretical physicist Phillip Wallace in 1947 [4]. Graphene is the two-dimensional (2D) building block which, when layered, constructs three-dimensional (3D) graphite, or pencil lead (Fig. 1.1).

Since its isolation, graphene, a semimetal, has been shown to exhibit some remarkable properties. For one, it is the strongest material that has ever been discovered; free-standing pristine graphene has an intrinsic tensile strength of 42 N/m [5]. This is a measurement of the tension required to break the film along one direction. Despite such strength, as a purely 2D material graphene is highly flexible. In addition, the charge carriers have the highest room-temperature mobility ever observed at about 200,000 cm$^2$/V·s [6], which is a measure of the reaction to an applied electric field in the charge carriers’ drift velocity. These properties, along with the ability to tune graphene’s optical response [7], give the material enormous potential in new technologies (flexible phones, efficient batteries, photovoltaic cells, etc. [8]). While the potential applications of graphene are appealing, perhaps more remarkable is the view of this material from a fundamental perspective.

Rather than behaving like typical electrons, the quasiparticles in graphene match the behaviour of massless Dirac fermions, with motion described by the Dirac equation [2,9,10]. This is what makes graphene a relativistic material, or more specifically, a relativistic Dirac material. These quasiparticles do not reach relativistic speeds (the Fermi velocity, $v_F$, of doped graphene is about $1 \times 10^6$ m/s [2], less than one percent the speed of light). However,
Figure 1.1: Graphene is the two-dimensional building block of the three-dimensional carbon material graphite, which is used as pencil lead.

their dynamics are the same as truly relativistic particles in a universe with an effective speed of light $v_F$. This is discussed with detail in Chapter 3.

Until 2004, experimental studies of massless Dirac fermions belonged only to the realm of high-energy physics. The variety of probes available to that field, however, are somewhat limited when compared to condensed matter. Graphene offers a table-top tunable system that can be examined using a versatile suite of instruments. For example, that Dirac fermions exhibit Klein tunnelling was not confirmed until it was first seen in graphene [11, 12]. This is the effect (thought previously to be a paradox in Dirac’s theory) whereby a massless Dirac fermion encountering a potential barrier at normal incidence will tunnel through unimpeded. There have also been strides toward an observation of zitterbewegung in graphene, the ‘wiggling motion’ that Dirac fermions are meant to exhibit (an oscillatory term in the time-dependent position operator) [13, 14]. This is where, in addition to there being a linear-in-time term, the position operator for a Dirac fermion has a term that oscillates.

The excitement surrounding graphene has led many to seek out other relativistic materials. One very large development has been in the study of topological insulators [15]. These are bulk insulators that host relativistic quasiparticles on their boundaries (i.e., edge
states in 2D or surface states in 3D materials). Other, more recent, developments have focused on variants of graphene based on the property of pseudospin. In addition to having the intrinsic spin of the electron, quasiparticles in relativistic materials are imbued with an emergent spin angular momentum (pseudospin). This is not merely a spin analogue like nuclear isospin, but in fact a real angular momentum [16]. In graphene, the pseudospin has a value of $s = 1/2$ whereby the two pseudospin projections ($\pm 1/2$) refer to the two triangular sublattices which make up graphene’s hexagonal honeycomb lattice.

Several hypothetical physical systems exhibiting various values of pseudospin have been proposed. Lan, Goldman, Bermudez, Lu, and Öhberg [17] outline a potential method to simulate Dirac fermions in 2D square optical lattices of ultracold atoms. This is achieved by tuning a spin-dependent laser-assisted hopping potential which is specific to the spin-$s$ representation of the SU(2) Lie algebra. In another theoretical construction, Dóra, Kailasvuori, and Moessner (DKM) [18] stack $2s + 1$ triangular sublattices and bond them in a particular way so as to create the 2D pseudospin-$s$ Dirac material. For the values $s = 1/2$ and $s = 1$, the DKM model constructs the graphene and dice lattices, respectively (the dice lattice is introduced in Chapter 3). The DKM construction of a Dirac material is purely geometric in that it relies only on the lattice configuration and does not require an external spin-dependent potential. It is possible to fabricate these arrays in photonic lattices or in the optical trapping of ultracold atoms [19]. In yet another theoretical design, Krishtopenko, Knap, and Teppe [20] describe the construction of an $s = 3/2$ 2D Dirac system which exists in a double HgTe/CdTe quantum well.

There are more exotic examples of higher-pseudospin systems. The edge-centred honeycomb lattice is an $s = 1/2$ Dirac material for filling fractions of $f = \{1/5, 4/5\}$, but for $f = 1/2$ is instead an $s = 1$ system [21]. The $\alpha$-$\mathcal{T}_5$ model [22] interpolates between the graphene honeycomb lattice and the dice lattice via a variable hopping parameter, allowing for a system that is an intermediate between (or hybrid of) the $s = 1/2$ and $s = 1$ system. This toy model has become quite popular with theorists in the brief period since it was conceived [23–28]. There are also 3D materials that have been shown to exhibit so-called massless Kane fermions [29–31], described by the low-energy Kane model for zinc-blende semiconductors under a particular set of parameters [32]. These massless Kane fermions are
relativistic in that they have linear-band single-point crossings, indicating zero mass excitations. When restricted to 2D, the massless Kane Hamiltonian maps onto the $\alpha$-$T_3$ model with $\alpha = 1/\sqrt{3}$ [24], demonstrating that the Kane fermion is a hybrid $s = 1/2$ and $s = 1$ Dirac fermion. Kane fermions are detailed in Chapter 3 and are the subject of Chapter 5.

The popularity of higher- or exotic-pseudospin relativistic materials motivates an in-depth theoretical study into their properties. Such an investigation is useful for comparing fundamental similarities and perhaps-novel differences in higher-pseudospin materials to the elementary $s = 1/2$ system in graphene. Additionally, an elaboration of material properties from a theoretical perspective can either direct the pursuits of experimentalists or confirm their results. In particular, at this early stage, properties which may provide unique signatures in experiment are useful in the potential discovery and identification of new relativistic materials. Such is the main concern of this thesis.

Many experiments involve the probing of a physical system and measuring a response. An optical absorption experiment is a good example. A beam of light acts as an external probe which induces a current in the material. The strength of this response at various frequencies is evident in the absorbance spectrum, which measures the reduction in the intensity of light after it passes through the material. The susceptibility of a material to some type of external stimulus (light, charge impurity, etc.) is useful to determine in that it only depends on the material properties and can be revealing of fundamental quasiparticle dynamics. Susceptibility is represented by a response function. In the example above, optical conductivity is the response function which describes the material’s susceptibility to an incident beam of light.

The response functions (optical conductivity and the dielectric function) of various relativistic systems are investigated from a theoretical perspective in subsequent chapters. These quantities do not only lend themselves as useful tools to experiment. In addition, they contain fundamental information on the band structure and dynamics of the system. By deriving analytic expressions for response functions, we obtain a good deal of insight into these systems and their novel properties, more than can be surmised from the band structure alone.

In Chapter 2, the mathematics behind linear response theory is detailed, with a focus on
optical conductivity, the dielectric function, and how these fit into experiment. Chapter 3 describes the various relativistic condensed matter systems discussed throughout the thesis and how they relate to the Dirac equation.

In Chapter 4, a derivation and detailed analysis of the magneto-optical conductivity of Dirac materials in 2D for all values of pseudospin-$s$ is provided. Continuous energy bands condense into highly degenerate discrete Landau levels. This creates unique structures in the optical conductivity, which demonstrates optically activated quantum transitions between levels. With the aid of so-called ‘snowshoe diagrams,’ these structures can be identified in optical spectra and act as signatures for each pseudospin-$s$ system. A similar magneto-optical analysis is then performed for the Kane model in Chapter 5 which is used to calculate the absorbance in the material Hg$_{1-x}$Cd$_x$Te.

In Chapter 6, an analytic expression for the polarizability of the 2D $s = 1$ Dirac system is derived. This is equivalent to a derivation of the dielectric function, which essentially contains all of the electronic information on the system. The dielectric function renormalizes the ordinary Coulomb potential between charges (screening) and describes any collective behaviour of the charge carriers (such as plasmon oscillations). The $s = 1$ system is particularly interesting because it bears host to a completely flat band, fixed at zero energy. The singular density of states found in the flat band lends an enormous amount of screening against an electronic mode with energy equal to the chemical potential. Finally, Chapter 7 briefly concludes the thesis.
Chapter 2

Response Functions

This chapter provides the mathematical background on response functions required for the original research presented in subsequent chapters. The information presented in this chapter relies heavily on Refs. [33–39], which are cited once here rather than being repeatedly referenced throughout.

In a typical experiment, a condensed matter system is probed with some perturbation (such as a beam of light) and the response to this stimulus is measured. The optical conductivity, polarizability, and dielectric function all include information about the system’s susceptibility to a general electromagnetic perturbation. These quantities depend only on material properties (not the specifics of the perturbation). In what follows, these quantities and their properties are rigorously defined. A connection is then made to these and quantities such as absorption and reflectivity which are measured in experiment.

2.1 Linear Response Theory

The way that a condensed matter system responds to an experimental probe is revealing of some of that system’s fundamental attributes. The strength of graphene, for instance, can be found by applying mechanical stress using an atomic force microscope and measuring the deformation of the material [5]. In this section, the general theory is detailed for the response in some observable of a system to some small perturbation up to linear order.

In the Schrödinger picture of quantum mechanics, the time-behaviour of the state space
is based on the Schrödinger equation with some initial condition,

\[ i\hbar \partial_t |a(t)\rangle = \hat{H}|a(t)\rangle, \quad |a(t_0)\rangle \equiv |a_0\rangle, \quad (2.1) \]

where \( \hat{H} \) is the system Hamiltonian operator. This equation has solution \( |a(t)\rangle = \hat{U}(t - t_0)|a_0\rangle \), where the time-evolution operator is

\[ \hat{U}(t - t_0) = \exp \left[ -i\frac{\hat{H}}{\hbar}(t - t_0) \right]. \quad (2.2) \]

Now suppose the Hamiltonian depends on time and can be split up into an equilibrium piece and a time-dependent interaction term,

\[ \hat{H}(t) = \hat{H}_0 + \hat{V}(t). \quad (2.3) \]

The interaction picture of quantum mechanics defines its state functions in terms of those in the Schrödinger picture,

\[ |a_I(t)\rangle = e^{i\frac{\hat{H}_0}{\hbar}t}|a(t)\rangle. \quad (2.4) \]

Using these states requires a new definition for operators. To see this, consider the expectation value of a general (Schrödinger) operator \( \hat{A}(t) \),

\[ \langle a(t)|\hat{A}(t)|a(t)\rangle = \langle a_I(t)|e^{i\frac{\hat{A}_0}{\hbar}t}\hat{A}(t)e^{-i\frac{\hat{A}_0}{\hbar}t}|a_I(t)\rangle. \quad (2.5) \]

Then operators in the interaction picture must be defined as

\[ \hat{A}_I(t) = e^{i\frac{\hat{A}_0}{\hbar}t}\hat{A}(t)e^{-i\frac{\hat{A}_0}{\hbar}t}. \quad (2.6) \]

The reason for using the interaction picture is in the time behaviour of the new state, which
depends only on the interaction $\hat{V}_I$,

$$i\partial_t|a_I\rangle = \partial_t\left(e^{i\hat{H}_0 t}|a(t)\rangle\right)$$
$$= e^{i\hat{H}_0 t}\left(\hat{H} - \hat{H}_0\right)|a(t)\rangle$$
$$= e^{i\hat{H}_0 t}V(t)e^{-i\hat{H}_0 t}|a_I(t)\rangle$$
$$= V_I(t)|a_I(t)\rangle , \tag{2.7}$$

The time-evolution operator in the interaction picture does not necessarily depend on the difference $t - t_0$,

$$|a_I(t)\rangle = \hat{U}_I(t, t_0)|a_I(t_0)\rangle . \tag{2.8}$$

Equation (2.7) gives the differential equation

$$i\partial_t \hat{U}_I(t, t_0) = \hat{V}_I(t)\hat{U}_I(t, t_0) \quad \hat{U}_I(t_0, t_0) = 1 . \tag{2.9}$$

Upon integration, a self-consistent equation is obtained for $\hat{U}_I$,

$$\hat{U}_I(t, t_0) = 1 - i \int_{t_0}^{t} dt'\hat{V}_I(t')\hat{U}_I(t', t_0) . \tag{2.10}$$

In a self-consistent manner, plugging the left-hand side into the right-hand side gives an approximation for the operator up to linear order in the interaction $\hat{V}(t)$,

$$\hat{U}_I(t, t_0) = 1 - i \int_{t_0}^{t} dt'\hat{V}_I(t') + \mathcal{O}(\hat{V}^2) . \tag{2.11}$$

Up to a factor equal to the partition function $Z$, the thermodynamic average of an operator $\hat{A}$ is equal to

$$\langle \hat{A}(t) \rangle = \sum_a e^{-\beta\varepsilon_a}\langle a_I(t)|\hat{A}(t)|a_I(t)\rangle$$
$$= \sum_a e^{-\beta\varepsilon_a}\langle a_I(t_0)|\hat{U}_I^\dagger(t, t_0)\hat{A}(t)\hat{U}_I(t, t_0)|a_I(t_0)\rangle . \tag{2.12}$$
Plugging in Eq. (2.11),

\[
\langle \hat{A}(t) \rangle = \sum_a e^{-\beta a} \langle a_I(t_0) | \hat{A}_I(t) | a_I(t_0) \rangle \\
\quad - i \int_{t_0}^{t} dt' \sum_a e^{-\beta a} \langle a_I(t_0) | [\hat{A}_I(t) \hat{V}(t') - \hat{V}(t') \hat{A}_I(t)] | a_I(t_0) \rangle + \mathcal{O}(\hat{V}^2) \\
= \langle \hat{A} \rangle_0 - i \int_{t_0}^{t} dt' \langle [\hat{A}(t), \hat{V}(t')] \rangle_0 + \mathcal{O}(\hat{V}^2),
\]

(2.13)

where \( \langle x \rangle_0 \) is an average over the equilibrium states since \( |a_I(t_0)\rangle = |a(t_0)\rangle \) is an eigenstate of \( \hat{H}_0 \).

\( \hat{V}(t) \) can represent a probe on the system, such as a beam of light onset at time \( t_0 \),

\[
\hat{V}(t) = \Theta(t - t_0) \hat{H}',
\]

(2.14)

where \( \Theta(x) \) is the Heaviside step function,

\[
\Theta(x) = \begin{cases} 
0 & x \leq 0 \\
1 & x > 0 
\end{cases}.
\]

(2.15)

From Eq. (2.12),

\[
\delta \langle \hat{A}(t) \rangle \equiv \langle \hat{A}(t) \rangle - \langle \hat{A} \rangle_0 = \int_{t_0}^{\infty} dt' C^+_{\hat{A}, \hat{H}'}(t, t'),
\]

(2.16)

which is written in terms of the retarded correlation function,

\[
C^+_{X_1, X_2}(t, t') = -i \Theta(t - t') \langle [X_1(t), X_2(t')] \rangle_0.
\]

(2.17)

Equation (2.16) is the general Kubo formula [40], giving the linear response in \( \hat{A} \) to the probe \( \hat{H}' \).
2.2 Kramers-Kronig Relation

The retarded correlation function in Eq. (2.17) obeys the rule of causality, owing to the fact that it is zero for $t < t'$. Causality, of course, should be expected in a quantity that describes a system’s response to some stimulus. In general, a causal function $\chi(t) = 0$ for all $t < 0$. After Fourier transform, this simple definition appears as a less-than-obvious relation in the frequency domain, arrived at independently by Kronig in 1926 [41] and Kramers in 1927 [42].

The Fourier transform of $\chi(t)$ gives

$$\chi(t) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \chi(\omega) .$$

For $t < 0$, where $\chi(t)$ is zero, Eq. (2.18) can be evaluated as a contour integral closed in the upper half of the complex-$\omega$ along a semicircle with radius $R \to \infty$ (Fig. 2.1(a))), which assumes $\omega > 0$. The factor $e^{-i\omega t}$ makes it so that the semi-circular piece at infinity does not contribute to the contour integral, leaving only the integration along the real axis in Eq. (2.18). Since $\chi(t < 0)$ is zero by definition, the full contour integral must be zero,

$$\chi(t < 0) = \oint_{C_a} d\omega e^{-i\omega t} \chi(\omega) = 0 .$$

Figure 2.1: (a) Contour $C_a (R \to \infty)$ used to evaluate the integral in Eq. (2.18). (b) Contour $C_b (R \to \infty)$ used in evaluating Eq. (2.20) which skips over the pole at $\omega = \nu$. 

(a) $\text{Im } \omega$ \hspace{2cm} (b) $\text{Im } \omega$
In order for Eq. (2.19) to be identically zero, there can be no poles enclosed by $C_a$. That is, $\chi(\omega)$ must be analytic everywhere in the upper-half of the complex plane.

Given the analyticity of $\chi(\omega)$ (no poles for $\text{Im } \omega > 0$ and $\chi(\omega) \to 0$ as $|\omega| \to \infty$), consider now the contour integral

$$\oint_{C_b} d\omega \frac{\chi(\omega)}{\omega - \nu} = 0,$$

where the contour $C_b$ (Fig. 2.1) is the same as $C_a$ except that it makes an infinitesimal hop around the pole at $\omega = \nu$. There are no poles contained by the contour, forcing the resulting integral to be zero. The large semi circle at infinity makes no contribution, while skipping around $\omega = \nu$ provides a term equal to $-i\pi \chi(\nu)$. Then Eq. 2.20 becomes

$$i\pi \chi(\nu) = \int_{-\infty}^{\infty} d\omega \mathcal{P} \frac{\chi(\omega)}{\omega - \nu},$$

where $\mathcal{P}$ denotes the principal part. This is defined so that for a function $f(x)$ which is singular at $x = a$, an integral of the principal value of $f(x)$ along the real axis is

$$\int_{-\infty}^{\infty} dx \mathcal{P} f(x) = \lim_{\eta \to 0} \left( \int_{-\infty}^{-\eta} dx f(x) + \int_{a+\eta}^{\infty} dx f(x) \right).$$

Equation (2.21) relates the real and imaginary parts of $\chi$ (written $\chi_1$ and $\chi_2$, respectively),

$$\chi_1(\nu) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \mathcal{P} \frac{\chi_2(\omega)}{\omega - \nu},$$

$$\chi_2(\nu) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \mathcal{P} \frac{\chi_1(\omega)}{\omega - \nu}.$$

This pair of equations is referred to as the Kramers-Kronig relation and applies to the Fourier transform of all causal functions $\chi(t)$. It is the manifestation of causality as it appears in the frequency domain.

If the response function in the time domain $\chi(t)$ is real, then it must be that $\chi(\omega) = \chi^*(-\omega)$. To see this, take the complex conjugate of Eq. (2.18),

$$\chi^*(t) = \int_{-\infty}^{\infty} d\omega e^{i\omega t} \chi^*(\omega) = \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \chi^*(-\omega).$$
Insisting that $\chi^*(t) = \chi(t)$ gives the result $\chi(\omega) = \chi^*(-\omega)$. This identity means that $\chi_1$ is an even function about $\omega = 0$ and $\chi_2$ an odd function. Then the integration domain in Eq. (2.23) can be reduced to positive values of $\omega$ only by multiplying each integrand by $\omega + \nu$ in both numerator and denominator, keeping only the even term in each integrand,

$$
\begin{align*}
\chi_1(\nu) &= \frac{2}{\pi} \int_0^\infty d\omega \mathcal{P} \frac{\omega \chi_2(\omega)}{\omega^2 - \nu^2}, \\
\chi_2(\nu) &= -\frac{2}{\pi} \int_0^\infty d\omega \mathcal{P} \frac{\nu \chi_1(\omega)}{\omega^2 - \nu^2}.
\end{align*}
$$

(2.25)

Finally, subtracting the singularity at $\omega = \nu$ from each integrand removes the need to evaluate the principal part,

$$
\begin{align*}
\chi_1(\nu) &= \frac{2}{\pi} \int_0^\infty d\omega \frac{\omega \chi_2(\omega) - \nu \chi_2(\nu)}{\omega^2 - \nu^2}, \\
\chi_2(\nu) &= -\frac{2}{\pi} \int_0^\infty d\omega \frac{\nu[\chi_1(\omega) - \chi_1(\nu)]}{\omega^2 - \nu^2}.
\end{align*}
$$

(2.26)

### 2.3 Optical Conductivity

In an optical measurement, a beam of light perturbs the system and elicits some measurable response. For transverse fields, the scalar potential is zero, $\varphi = 0$. As such, light is described solely by the vector potential, $A$. At leading order, it couples with the current, $j$, via the perturbation

$$
\hat{\mathcal{H}}' = -\frac{1}{c} \int d^d r \mathbf{j} \cdot \mathbf{A}(r).
$$

(2.27)

From Eq. (2.16), the response in the current is

$$
\delta\langle j(t) \rangle = -i \int_{-\infty}^t dt' \langle [\mathbf{j}(t), \hat{\mathcal{H}}'(t')] \rangle,
$$

(2.28)

where it is assumed that the onset of the perturbation occurred sufficiently far in the past ($t_0 \to -\infty$). Inserting $\hat{\mathcal{H}}'$ into the commutator,

$$
\delta\langle j_{\alpha}(t) \rangle = i \int_{-\infty}^t dt' \langle [j_{\alpha}(t), j_{\beta}(t')] \rangle A_{\beta}(t').
$$

(2.29)

When working at linear order, it is fine to assume that the light is monochromatic,
described by an electric field \( \mathbf{E}(t) = \mathbf{E}_0 e^{-i\omega t} \). Any additional modes can be included simply by linear superposition. As such, the vector potential is expressed via

\[
\mathbf{E} = -\partial_t \mathbf{A} \implies \mathbf{A} = \frac{1}{i\omega} \mathbf{E}.
\] (2.30)

This leads to the material’s susceptibility in the current to the incident electric field,

\[
\delta \langle j_\alpha(t) \rangle = \int_{-\infty}^{\infty} dt' \sigma_{\alpha\beta}(t, t') E_\beta(t') + O(E^2),
\] (2.31)

which serves as the definition of the optical conductivity tensor, \( \sigma_{\alpha\beta} \). Optical conductivity measures the first-order susceptibility of a system to some optical probe and involves the retarded current-current correlation function,

\[
\sigma_{\alpha\beta}(t, t') = \frac{i}{\omega} C^+_{j\alpha j\beta}(t, t').
\] (2.32)

The analysis of two-point correlation functions is typically done using the quantum many-body Green’s functions approach. This perturbative method is well established, but rather involved, requiring several lengthy definitions before one can finally arrive at the result. As such, it is not detailed here. Instead the reader is directed to Refs. [34,37] for the standard presentation as it applies to condensed matter. The derivation of the correlation function is most easily performed in the frequency domain, \( \omega \), arrived at through a Fourier transform. The resulting expression for the conductivity involves matrix elements of the equilibrium current operator, \( \hat{j} = \partial \hat{\mathcal{H}}_0 / \partial \mathbf{k} \), and the Fermi-Dirac distribution, \( n_f(x) = (1 + e^{-(x-\mu)/k_B T})^{-1} \), which in turn depends on the chemical potential \( \mu \) and thermal energy \( k_B T \). The expression is

\[
\sigma_{\alpha\beta}(\omega) = ig \sum_\mathbf{k} \sum_{a,b} n_f(\varepsilon_a(\mathbf{k})) - n_f(\varepsilon_b(\mathbf{k})) \frac{\langle a(\mathbf{k})|j_a(\mathbf{k})\rangle \langle b(\mathbf{k})|j_b(\mathbf{k})\rangle}{\varepsilon_b(\mathbf{k}) - \varepsilon_a(\mathbf{k})} \frac{\hbar \omega - (\varepsilon_b(\mathbf{k}) - \varepsilon_a(\mathbf{k})) + i\eta}{\hbar^2 \omega}.
\] (2.33)

where \( g \) is a degneracy factor and \( \eta = 0^+ \) can be interpreted as an infinitesimal scattering rate of the energy eigenstates. The sum over \( \mathbf{k} \) represents a full trace over the parameter space on which the bands, \( |a\rangle \), and corresponding energy dispersions, \( \varepsilon_a \), depend.
The real and imaginary parts of the conductivity can be separated using the identity
\[
\lim_{\eta \to 0^+} \frac{1}{x + i\eta} = \mathbb{P} \frac{1}{x} - i\pi \delta(x),
\]
where \(\delta(x)\) is the Dirac-delta function. For a longitudinal component of the conductivity \((\alpha = \beta)\),
\[
\text{Re} \sigma_{\alpha\alpha}(\omega) = \frac{g\pi}{\omega} \sum_k \sum_{a,b} \Delta n_f |\langle a|\hat{j}_\alpha|b\rangle|^2 \delta(\omega - \Delta \varepsilon),
\]
\[
\text{Im} \sigma_{\alpha\alpha}(\omega) = g \sum_k \mathbb{P} \sum_{a,b} \frac{\Delta n_f |\langle a|\hat{j}_\alpha|b\rangle|^2}{\omega - \Delta \varepsilon},
\]
where the notation in Eq. (2.33) has been simplified by using the symbols \(\Delta n_f = n_f(\varepsilon_a) - n_f(\varepsilon_b)\) and \(\Delta \varepsilon = \varepsilon_b - \varepsilon_a\) and taking photon energy to be \(\omega\) (rather than \(\hbar \omega\)). We observe that the summand in the real part is proportional to the probability density that a photon of energy \(\omega\) activates a transition between the state \(|b\rangle\) and \(|a\rangle\) (or vice versa) while obeying the conservation of energy. The \(\Delta n_f\) factor ensures that one of these states is filled and the other occupied so that the transition promotes a particle into a hole state. The delta function is zero for transitions that do not obey energy conservation, making the real part an ‘on-shell’ quantity. As such, \(\text{Re} \sigma_{\alpha\alpha}\) is referred to as the absorptive part of the longitudinal conductivity. The imaginary part, being ‘off-shell,’ is referred to as the reactive part. The opposite is true for the transverse conductivity \(\sigma_{\alpha\phi}\) (where \(\phi\) is the complement of \(\alpha\)). Because the product of transverse matrix elements in Eq. (2.33) is purely imaginary, it is \(\text{Im} \sigma_{\alpha\phi}\) that is absorptive and \(\text{Re} \sigma_{\alpha\phi}\) reactive for the transverse conductivity.

2.4 The Dielectric Function and Polarizability

The high density of charge carriers in a condensed matter system has the ability to screen the typical electronic interaction between charged species separated by vacuum. The potential, as it exists outside of the system, is renormalized to a new form inside of the material. The effects of this renormalization are referred to as the dielectric properties of the material.

We assume that the vacuum interaction is described by the bare Coulomb potential
energy between two $-e$ charges,

$$V_c(r) = \frac{\alpha \hbar c}{r},$$  \hspace{1cm} (2.36)

where $\alpha$ is the ratio between the vacuum Coulomb energy per particle and the average kinetic energy per particle in the system. It plays the role of an effective fine structure constant. In a vacuum, the fine structure constant is $\alpha = e^2/\epsilon_0 \hbar c \approx 1/137$, where $\epsilon_0$ is the permittivity of free space.

The screened interaction will be a renormalization of the Coulomb interaction,

$$V(r) = \int d^d r' \epsilon^{-1}(r,r')V_c(r').$$  \hspace{1cm} (2.37)

where $\epsilon$ is the (dimensionless) dielectric function, or relative permittivity, which can generally depend on space and time. Its inverse, $\epsilon^{-1}$, is defined by the direct-space integral

$$\int d^d r' \epsilon^{-1}(r,r') \epsilon(r',r'') = \delta^d(r-r').$$  \hspace{1cm} (2.38)

This identity simplifies greatly in reciprocal space, where differential equations become algebraic,

$$\epsilon^{-1}(q) = \frac{1}{\epsilon(q)}. \hspace{1cm} (2.39)$$

Note that the averaging over space by the measure $\int d^d r'$ requires division by the total volume of the system which is not explicitly written here.

The dielectric nature of the condensed matter system will induce a change in the system's total scalar potential $\varphi$ relative to an external potential, $\varphi_0$,

$$\varphi(r,t) = \int d^d r' dt' \epsilon^{-1}(r,t;r',t') \varphi_0(r',t').$$  \hspace{1cm} (2.40)

These two quantities have a source-and-response interaction with $\epsilon^{-1}$ playing the role of the susceptibility. As such, linear response theory (Eq. (2.16)) can be used to derive an expression for the dielectric function.
The perturbation on the system from $\varphi_0$ is

$$\hat{\mathcal{H}}'(t) = \int d^d r \rho(r,t) \varphi_0(r,t), \quad (2.41)$$

where $\rho$ is charge density. Then, from the Kubo formula in Eq. (2.16), the leading-order induced charge density is

$$\delta \langle \rho \rangle = \int d^d r' dt' C_{\rho,\rho}^+(r,t;r',t') \varphi_0(r',t') + O(\varphi_0^2). \quad (2.42)$$

The susceptibility of the charge density to $\varphi_0$ is referred to as the reducible polarizability, $Q_R$, and is equal to the retarded density-density correlation function,

$$Q_R(r,t;r',t') \equiv C_{\rho,\rho}^+(r,t;r',t') = -i \Theta(t-t') \langle [\rho(r,t),\rho(r',t')] \rangle_0. \quad (2.43)$$

The ‘reducible’ description comes from the many-body Green’s function technique. The calculation of $Q_R$ involves the summation of Feynman diagrams (shorthand diagrams representing rather involved integrals). Many of the terms in the sum are made up of irreducible diagrams connected together. Later in the derivation, Dyson’s formula is applied so that the result is based on the irreducible polarizability, $Q$ (simply referred to as the polarizability). $Q$ involves a summation of only the irreducible Feynman diagrams that appear in $Q_R$ and does not include their infinitely many reducible terms. Again, the reader is referred to Refs. [34,37] for details on the many-body Green’s function approach.

Based on the induced charge distribution, the induced potential in the system is

$$\delta \langle \varphi(r) \rangle = \int d^d r' V_c(r-r') \delta \langle \rho(r') \rangle. \quad (2.44)$$

Then the total potential in the system is

$$\langle \varphi(r,t) \rangle = \varphi_0 + \delta \langle \varphi \rangle$$

$$= \varphi_0(r,t) + \int d^d r' d^d r'' dt' V(r-r')Q_R(r',t;r'',t'). \quad (2.45)$$
The inverse dielectric function is read off from Eq. (2.40) as

$$\epsilon^{-1}(r, t; r', t') = \delta^d(r - r')\delta(t - t') + \int d^dr''V_c(r - r'')Q(r'', t; r', t'). \quad (2.46)$$

Making a Fourier transform into the momentum and frequency domains gives a more tractable form,

$$\epsilon^{-1}(q, \omega) = 1 + V_c(q)Q^R(q, \omega). \quad (2.47)$$

The Coulomb potential in momentum space depends on the dimensionality of the system. For example, in 2D and 3D, respectively,

$$V_c(q) = \frac{2\pi\alpha\hbar c}{q} \quad (2D),$$

$$V_c(q) = \frac{4\pi\alpha\hbar c}{q^2} \quad (3D). \quad (2.48)$$

The reducible and irreducible polarizabilities are related via (not derived here),

$$Q^R(q) = \frac{-Q(q)}{1 + V_c(q)Q(q)}. \quad (2.49)$$

Plugging this into Eq. (2.47) gives the dielectric function in terms of the irreducible polarizability,

$$\epsilon(q, \omega) = 1 + V_c(q)Q(q, \omega). \quad (2.50)$$

The result for the polarizability under the random-phase approximation (RPA) is

$$Q(q, \omega) = g \sum_k \sum_{a,b} \frac{n_f(\varepsilon_a(k')) - n_f(\varepsilon_b(k))}{\hbar\omega - (\varepsilon_a(k') - \varepsilon_b(k)) + i\eta} |\langle a(k')|b(k)\rangle|^2, \quad (2.51)$$

where $k' = q + k$. The RPA is an approximation where, in the Feynman-diagram representation, the polarizability is taken to be the particle-hole bubble (mathematically expressed by Eq. (2.51)). Higher-order diagrams are excluded which involve interactions occurring within the bubble, corresponding to terms like $|\langle a|V|b\rangle|^2$. The term ‘random-phase’ is remnant of an equivalent procedure employed by Bohm and Pines that pre-dates the advent of many-body Green’s functions [43].
Using the identity in Eq. (2.34),

\[
\text{Re} \ Q(q, \omega) = g \sum_k P \sum_{a,b} \frac{n_f(\varepsilon_a(k')) - n_f(\varepsilon_b(k))}{\hbar \omega - (\varepsilon_a(k') - \varepsilon_b(k))} |\langle a(k')|b(k)\rangle|^2 ,
\]

\[
\text{Im} \ Q(q, \omega) = g \sum_k \sum_{a,b} [n_f(\varepsilon_a(k')) - n_f(\varepsilon_b(k))] |\langle a(k')|b(k)\rangle|^2 \delta(\hbar \omega - (\varepsilon_a(k') - \varepsilon_b(k))).
\]

(2.52)

As the on-shell piece of density-density correlator, \text{Im} \ Q maps out the particle-hole continuum (PHC). This is the region in \((q, \omega)\)-space where \text{Im} \ Q is non-zero, demonstrating a geometric connection between particle and hole states that are separated by momentum \(\hbar q\) and energy \(\hbar \omega\). Outside of the PHC, it is impossible to scatter a particle into a hole state.

Consider now the macroscopic Maxwell equations. The electric field, \(E\), and the displacement field in the system, \(D\), are related by

\[
D(q, \omega) = \epsilon(q, \omega) \epsilon_0 E(q, \omega).
\]

(2.53)

The wave equation for radiation in the material (assumed isotropic and non-magnetic) is

\[
\mu_0 \partial_t^2 D(r, t) = \nabla^2 E(r, t),
\]

(2.54)

where \(\mu_0\) is the permeability of free space. Suppose the electric field is a plane wave \(E \sim e^{i(q \cdot r - \omega t)}\). Then the wave equation above leads to the relation

\[
\frac{\omega^2}{c^2} \epsilon(q, \omega) = q^2.
\]

(2.55)

Thus \(q \sim \sqrt{\epsilon}\). Different cases based on the nature of \(\epsilon(q, \omega)\) arise,

\begin{itemize}
  \item \(\text{Re} \ \epsilon < 0\) and \(\text{Im} \ \epsilon = 0\). Here \(q\) is imaginary, leading to an evanescent wave in the medium which decays over a length scale similar to \(1/q\).
  \item \(\text{Re} \ \epsilon > 0\) and \(\text{Im} \ \epsilon = 0\). Here \(q\) is real, allowing for the unattenuated propagation of electromagnetic radiation.
  \item \(\text{Re} \ \epsilon \neq 0\) and \(\text{Im} \ \epsilon \neq 0\) in general. Here \(q\) is complex, so that attenuated radiation is
\end{itemize}
present.

- $|\epsilon| \rightarrow \infty$. In this case, the displacement field $D$ exhibits an internal response in the absence of the field $E$. This region in $(q, \omega)$ space traces out the system’s quasiparticle energy dispersion.

- $\epsilon = 0$. This value allows for the propagation of longitudinal electromagnetic radiation through the system, which exhibits a corresponding oscillation of the charged medium (or plasma). The fundamental quantum of the collective plasma oscillation is referred to as a \textit{plasmon}.

The plasmon energy dispersion $\epsilon_p = \hbar \omega_p(q)$ is defined by zeros of the dielectric function,

$$
\epsilon(q, \omega_p - i\eta_p) = 0, \quad \text{(2.56)}
$$

where $\eta_p$ is the plasmon decay rate. Expanding this equation about small values of $\eta_p$ gives

$$
0 = 1 + V_c(q)Q(q, \omega_p) - i\eta_pV_c(q)\partial_\omega Q(q, \omega_p) + O(\eta_p^2). \quad \text{(2.57)}
$$

At leading order, the real part of Eq. (2.57) provides an expression for $\omega_p(q)$ (which is typically solved numerically),

$$
0 = q + 2\pi\alpha\text{Re } Q(q, \omega_p). \quad \text{(2.58)}
$$

The imaginary part gives the decay rate,

$$
\eta_p = \frac{\text{Im } Q(q, \omega_p)}{\partial_\omega \text{Re } Q(q, \omega_p)}. \quad \text{(2.59)}
$$

Then $\eta_p$ is smallest in regions where Im $Q$ is small, making Eq. (2.58) most accurate outside of the particle-hole continuum. Inside of the PHC, especially near a pole, plasmonic behaviour is heavily damped by the creation of particle-hole pairs.
2.5 Connection to Experiment

From the charge continuity equation,

\[ \partial_t \rho(r, t) + \nabla \cdot j(r, t) = 0, \]  

it can be shown that the optical conductivity and the dielectric function are not independent. Working in the \((q, \omega)\)-domain, using the definition of the conductivity in Eq. (2.31), and assuming an isotropic geometry so that \(\sigma_{\alpha\beta} = \sigma \mathbb{1}\), the continuity equation becomes

\[ -i\omega \rho(q, \omega) + i\sigma(q, \omega)q \cdot E(q, \omega) = 0. \]  

By working in the Coulomb gauge, \(q \cdot A = 0\) so that the definition \(E = -\nabla \varphi_0 - \partial_t A\) leads to

\[ -i\omega \rho(q, \omega) + q^2 \sigma(q, \omega)\varphi_0(q, \omega) = 0. \]  

Using the polarizability as defined in Eqs. (2.42) and (2.43) and subsequently comparing factors on \(\varphi_0\), we obtain

\[ Q^R(q, \omega) = \frac{q^2}{i\omega} \sigma(q, \omega). \]  

Finally, multiplying by \(V_c\) and adding 1 to both sides gives the desired relationship,

\[ \epsilon^{-1}(q, \omega) = 1 - \frac{iq^2}{\omega}V_c(q)\sigma(q, \omega). \]  

Equipped with either the dielectric function or optical conductivity, one has the entire knowledge of a condensed matter system’s response to electric perturbations, and of the renormalized interactions within the system. However, \(\epsilon\) and \(\sigma\) are not always immediately accessible to experimentalists. Certain measurements may reveal components of these functions (maybe real or imaginary part only over a limited range of energy). The Kramers-Kronig relation can then be employed to determine the missing components.
Table 2.1: Pairs of quantities which obey the Kramers-Kronig relation in Eq. (2.26).

<table>
<thead>
<tr>
<th>Quantity</th>
<th>χ₁</th>
<th>χ₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity</td>
<td>Re σ</td>
<td>Im σ</td>
</tr>
<tr>
<td>Polarizability</td>
<td>Re Q</td>
<td>Im Q</td>
</tr>
<tr>
<td>Dielectric Function</td>
<td>(Re ϵ - 1)</td>
<td>Im ϵ</td>
</tr>
<tr>
<td>Optical Constants</td>
<td>(˜n - 1)</td>
<td>˜k</td>
</tr>
<tr>
<td>Reflectivity</td>
<td>(\frac{1}{2} \ell \eta R)</td>
<td>θ</td>
</tr>
</tbody>
</table>

Recall that for a plane wave through the medium, \(E \sim e^{i(q \cdot r - \omega t)}\) (Eq. (2.54)),

\[ q = \frac{\omega}{c} \sqrt{\epsilon(q, \omega)}. \]  

(2.65)

We define the real and imaginary parts of \(\sqrt{\epsilon}\) as

\[ \sqrt{\epsilon} = \tilde{n} + i \tilde{k}, \]  

(2.66)

where \(\tilde{n}\) and \(\tilde{k}\) are the familiar index of refraction and extinction coefficient, referred to as the optical ‘constants’ (despite being allowed to vary in general). Based on these measurable quantities,

\[ \text{Re } \epsilon = \tilde{n}^2 - \tilde{k}^2, \quad \text{Im } \epsilon = 2\tilde{n}\tilde{k}. \]  

(2.67)

In an optical absorption experiment, a beam of light with initial intensity \(I_0\) is collected after passing through a medium over a distance \(d\), falling to an intensity \(I_a = I_0 e^{-\lambda d}\), where \(\lambda\) is the absorption coefficient. The attenuation of a beam of light through the medium is directly related to the extinction coefficient, giving

\[ \lambda = \frac{\omega \tilde{k}}{2c}. \]  

(2.68)

In another optical experiment, reflectivity measures the ratio of intensities of the incident and reflected beams, \(R = I_r / I_0\), off of a material surface, as well as the phase shift between

21
beams, $\theta$.

While two quantities are generally required to determine both the real and imaginary parts of $\varepsilon$ or $\sigma$, the Kramers-Kronig relation makes it so only one measurement over a sufficiently large enough range of frequency may be necessary. From Eq. (2.26) the integral determining $\chi_1(\nu)$ is dominated by the region $\omega \sim \nu$. If $\chi_2(\omega)$ is known in this region, then $\chi_1(\nu)$ can be determined with good accuracy (or vice versa). Many of the quantities discussed in this chapter are related by Eq. (2.26). These pairings are summarized in Table 2.1, which identify $\chi_1$ and $\chi_2$ in each pair.
Chapter 3

Relativistic Condensed Matter Systems

This chapter details the various relativistic condensed-matter systems investigated in subsequent chapters and their relevant properties.

3.1 The Dirac and Weyl Equations

The derivation of and solution to the Dirac equation is not provided here since it can be found in most quantum field theory texts [44]. However, it will at least be noted that Paul Dirac’s unification of quantum mechanics and special relativity in 1928 [45] is hugely important to the history of modern physics and is recognized as one of the major accomplishments in all of theoretical physics. In his equation, Dirac derived the property of particle spin and, without any precedence, predicted the existence of antiparticles. The equation forms the basis of the Standard Model of particle physics, and is now the linchpin in a booming branch of quantum condensed matter physics.

In the high-energy picture, the Dirac equation for a relativistic field, or spinor, $\psi(x)$, with mass $m$ in $(d+1)$-dimensional spacetime $x = x^\mu = (ct, \vec{x})$ is

$$\left(i\hbar \gamma^\mu \partial_\mu - mc\right)\psi(x) = 0,$$

(3.1)

where $a^\mu b_\mu$ is an innerproduct mediated by the Minkowski metric, $\eta^{\mu\nu} = \text{diag}(1, -1, ..., -1)$.
and \{\gamma^\mu\} is a set of \(d+1\) matrices that satisfy the Clifford algebra,

\[
\{\gamma^\mu, \gamma^\nu\} \equiv \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu}.
\] (3.2)

There is no unique solution to Eq. (3.2), but it can be shown that the minimum dimension of each matrix \(\gamma^\mu\) in a particular representation is \(N \times N\), where \(N = 2^{[(d+1)/2]}\) and \([x]\) is the floor of \(x\).

**Two Dimensions**

In 2+1 dimensions, where \(\eta^{\mu\nu} = \text{diag}(1, -1, -1)\), the Clifford algebra can be satisfied by the Pauli matrices: \(\gamma^\mu = (\sigma^z, i\sigma^y, -i\sigma^x)\), where

\[
\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\] (3.3)

Using this representation in Eq. (3.1), acting on the left with \(\sigma^z\), rearranging terms, and finally performing a Fourier transform into momentum space (so that \(i\hbar \partial \rightarrow \hbar \mathbf{k}\)), we obtain the form of the Dirac equation typically used for 2D condensed matter systems,

\[
i\hbar \partial_t \psi = (\hbar \bar{c} \sigma \cdot \mathbf{k} + m\bar{c}^2 \sigma^z) \psi,
\] (3.4)

where \(\sigma = (\sigma^x, \sigma^y)\), \(\mathbf{k} = (k_x, k_y)\), and \(c\) has been replaced with an effective speed of light, \(\bar{c}\), now that we have moved into the condensed-matter picture. Equation (3.4) is recognized as the Schrödinger equation with the operator on the right-hand side taking the role of the spin-1/2 massive Dirac Hamiltonian in 2D, where \(\hbar \sigma / 2\) is the spin-1/2 operator on \(\psi\).

In a condensed matter system, charge carriers are densely packed and interact in often intricate ways. The ground state of this ‘electron soup’ makes up, in the high-energy lexicon, the quantum vacuum of the system. A quantized single-particle excitation out of the ground state may be similar to an electron, or could very well be of a wholly different character. For example, this quasiparticle excitation might be described by relativistic Dirac physics, despite being in a non-relativistic system.
In the condensed matter picture, $\psi$ in Eq. (3.4) represents the spatial degrees of freedom in the quasiparticle wave function. The total quasiparticle wave function is $\Psi(\mathbf{x}) = \psi(\mathbf{x}) \otimes \chi_{1/2}$. The 2-spinor $\chi_{1/2}$ represents the intrinsic spin-1/2 of the electron that is carried onto quasiparticle excitations. When the remaining piece, $\psi$, then satisfies the Dirac equation (at least on some energy scale, as seen for the dice lattice in Section 3.4), it provides an additional spin structure to the full wavefunction $\Psi$. In order to avoid confusion with the intrinsic electron spin, $\chi_{1/2}$, this emergent piece is referred to as the pseudospin. Pseudospin is not merely a quantum spin analogue like nuclear isospin, but is, in fact, an additional spin angular momentum, as detailed by Mecklenburg and Regan [16].

Condensed matter arrangements bear host to countless various physical systems at low energy, each their own model universe [46]. There is no reason then to restrict pseudospin to the value of $s = 1/2$ in the way that intrinsic spin is. As such, we can generalize Eq. (3.4) to admit any value of pseudospin by replacing the Pauli matrices with the spin-$s$ matrices, $\{S^x, S^y, S^z\}$. This gives the 2D pseudospin-$s$ massive Dirac Hamiltonian,

$$\hat{\mathcal{H}}_D = \hbar v \mathbf{S} \cdot \mathbf{k} + mS^z,$$

where $v$ is a parameter with the dimension of velocity (in general $v$ is not the Fermi velocity). Based on spin states $|s, \lambda = \{-s, ..., s\}\rangle$, the matrix elements of the general pseudospin matrices are

$$
\langle \lambda' | S^x | \lambda \rangle = \frac{1}{2} \sqrt{s(s+1) - \lambda' \lambda (\delta_{\lambda', \lambda-1} + \delta_{\lambda', \lambda+1})},
$$
$$
\langle \lambda' | S^y | \lambda \rangle = \frac{i}{2} \sqrt{s(s+1) - \lambda' \lambda (\delta_{\lambda', \lambda-1} - \delta_{\lambda', \lambda+1})},
$$
$$
\langle \lambda' | S^z | \lambda \rangle = \lambda \delta_{\lambda', \lambda},
$$

where $\delta_{a,b}$ is the Kronecker delta. In terms of standard matrix indices $m$ and $n$ (which
range from 1 to \(2s+1\),

\[
S^x_{mn} = \frac{1}{2}(\rho_n\delta_{m,n+1} + \rho_m\delta_{n,m+1}),
\]
\[
S^y_{mn} = \frac{i}{2}(\rho_n\delta_{m,n+1} - \rho_m\delta_{n,m+1}),
\]
\[
S^z_{mn} = (s+1-m)\delta_{mn},
\]  

(3.7)

where \(\rho_m = \sqrt{m(2s+1-m)}\). Also relevant are the pseudospin raising and lowering operators \(S^\pm = S^x \pm iS^y\).

By setting the mass \(m = 0\) in Eq. (3.5), we obtain exactly the Weyl Hamiltonian,

\[
\hat{H}^s_W = \hbar v \mathbf{S} \cdot \mathbf{k}.
\]  

(3.8)

As such, the massless Dirac Hamiltonian in 2D is often referred to together as the Dirac-Weyl Hamiltonian. To be specific, Eq. (3.8) is one of the two chiral versions of the Weyl Hamiltonian. The opposite chirality is obtained by taking \(\mathbf{S} \rightarrow -\mathbf{S} \) (or \(-\mathbf{S}^*\)) and is physically manifest in the helicity of particles, represented by the operator \(h = \mathbf{S} \cdot \mathbf{k}/|\mathbf{S} \cdot \mathbf{k}|\) [13,44].

For a right-handed particle, the helicity is positive \((h = +1)\), meaning that its pseudospin points in the same direction as its momentum. A left-handed particle has negative helicity \((h = -1)\), so that pseudospin and momentum point in opposite directions. The reverse is true for right- and left-handed holes, or antiparticles: a right(left)-handed hole has negative (positive) helicity.

**Three Dimensions**

In 3 + 1 dimensions, a useful representation of the gamma matrices (referred to as the Weyl representation) leads to a particular form of the 3D pseudospin-s Dirac Hamiltonian,

\[
\hat{H}^s_D = \begin{pmatrix}
\hbar v \mathbf{S} \cdot \mathbf{k} & m \\
m & -\hbar v \mathbf{S} \cdot \mathbf{k}
\end{pmatrix},
\]  

(3.9)

with \(\mathbf{S} = (S^x, S^y, S^z)\) and \(\mathbf{k} = (k_x, k_y, k_z)\) now 3-vectors. The 2D massless Dirac equation is exactly the Weyl equation, whereas the 3D massless Dirac Hamiltonian \((m = 0)\) is a
4 × 4 object containing both the right- and left-chiral Weyl equations in block form along the diagonal. A finite mass mixes these two chiral sectors, but for \( m = 0 \), the Hamiltonian decomposes, making the sectors independent,

\[
\hat{H}^s_D\big|_{m=0} = \hat{H}^s_{W,r} \oplus \hat{H}^s_{W,\ell},
\]

where the \( r \) and \( \ell \) refer to the chirality of each sector.

Note that one must be aware of the number of dimensions in order to decide whether \( \hat{H}_D \) refers to Eq. (3.5) or Eq. (3.9), which give the 2D and 3D Dirac equations, respectively. On the other hand, Eq. (3.8) describes the Weyl equation in any dimension.

### 3.2 2D Weyl Fermions in a Magnetic Field

At zero magnetic field, the energy eigenvalues for the Weyl Hamiltonian in Eq. (3.8) are linear in momentum,

\[
\varepsilon_\lambda(k) = \lambda \hbar v k,
\]

where \( \lambda = \{-s, ..., s\} \) are pseudospin quantum numbers and \( k = \sqrt{k_x^2 + k_y^2} \) in 2D. This gives \( 2s + 1 \) conic bands in the energy dispersion that all touch at a single point, \( \varepsilon = k = 0 \), a special band crossing referred to as the Dirac point. The band dispersions for pseudospin values \( s = \{1/2, 1, 3/2, 2\} \) are plotted in Fig. 3.1. Each band in the figure is labelled with \( \lambda \). A positive chemical, \( \mu \), potential has been inscribed to each system in the figure, measured from the Dirac point to the Fermi surface (or Fermi ‘perimeter’ in 2D). \( \mu \) marks the divide between occupied (blue) and unoccupied (red) states. In addition to being the pseudospin-projection quantum number, \( \lambda \) defines the slope of each band, which in turn provides the band-specific Fermi velocity \( v_{f,\lambda} = |\partial_k \hat{H}| = |\lambda| \hbar v \). The finite-energy bands are often referred to as Dirac cones and the zero-energy band as the flat band.

For integer values of \( s \), an odd number of bands arise. Owing to the fact that the Weyl equation is particle-hole symmetric, this forces one of the bands to be pinned to zero energy (\( \lambda = 0 \)). The large degeneracy in this dispersionless, or flat, band leads to a singular density of states which can potentially give rise to interesting physical features.
Figure 3.1: Weyl energy dispersion for various pseudospin, $s$. The Fermi surface marks the divide between occupied (blue) and unoccupied (red) states. The pseudospin projection along the direction of momentum is indicated on each band. This number also dictates the slope of each band.
in a material. For example, highly degenerate Landau levels (LL’s), which form in the presence of a magnetic field, give rise to the fractional quantum Hall effect under partial filling \[47, 48\]. In addition, room-temperature superconductivity has been proposed as a possible feature of systems with flat-band surface states \[49\].

In the presence of an external magnetic field, the kinetic momentum \( \hbar \mathbf{k} \) is no longer conjugate to position. A Peierls substitution must be made, \( \hbar \mathbf{k} \rightarrow \hbar \mathbf{\Pi} = \hbar \mathbf{k} + e \mathbf{A}/c \), where \( \mathbf{A} \) is the vector potential associated with the field and \( \hbar \mathbf{k} \) now represents the canonical momentum \[13, 50\]. It is the canonical momentum that is conjugate to position, specified by the commutation relationship \([x, k_x] = [y, k_y] = i\).

In a 3D lab setting, a constant magnetic field is represented by a 3-vector, \( \mathbf{B} = \nabla \times \mathbf{A} = (0, 0, B) \), with the z-component pointing along the direction of the magnetic field by choice. This makes the Landau gauge convenient for representing the vector potential, \( \mathbf{A} = (-By/2, Bx/2, 0) \). Inside a 2D system situated in the \( xy \)-plane of the lab (unaware of the third dimension), the magnetic field is a scalar \( B = dA \). The cross-product from 3D must be generalized here to an exterior derivative \( dA = \epsilon^{\mu\nu} \partial_\mu A_\nu \), where \( \epsilon^{\mu\nu} \) is the totally antisymmetric matrix and \( \mathbf{A} = (-By/2, Bx/2) \) is now a 2-vector, appropriately matching the dimensionality of the confined space.

In the Landau gauge, the kinetic momentum is

\[
\begin{align*}
\hbar \mathbf{\Pi}_x &= \hbar k_x - \frac{eB}{2c} y, \\
\hbar \mathbf{\Pi}_y &= \hbar k_y + \frac{eB}{2c} x.
\end{align*}
\]

These two components obey the commutation relation

\[
[\mathbf{\Pi}_x, \mathbf{\Pi}_y] = \frac{eB}{2\hbar c} ([k_x, x] - [y, k_y]) = -\frac{i}{\ell_B^2},
\]

where \( \ell_B = \sqrt{\hbar c/eB} \) is the magnetic length scale, sometimes called the Larmor radius. This commutator prompts the construction of bosonic creation and annihilation operators

\[
a^\dagger = \frac{\ell_B}{\sqrt{2}} (\mathbf{\Pi}_x + i\mathbf{\Pi}_y), \quad a = (a^\dagger)^\dagger.
\]
These make up creation and annihilation, or Fock, operators strictly because their commutator is unity:

\[
[a, a^\dagger] = \frac{e^2_B}{2} \left( i[\Pi_x, \Pi_y] - i[\Pi_y, \Pi_x] \right) = 1.
\] (3.15)

What makes them bosonic is that a commutator is used; fermionic Fock operators obey an anticommutator relation. It can be shown from Eq. (3.15) that these operators act on a (bosonic) Fock space \( \mathcal{F} = \text{span}\{ |n\rangle, n \in \mathbb{Z}^* \} \), where \( \mathbb{Z}^* \) is the set of non-negative integers [39]. Their action on the vectors, or Landau levels, in this space is

\[
a|n\rangle = \sqrt{n}|n-1\rangle,
\]

\[
a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle,
\] (3.16)

with their product \( a^\dagger a \) being referred to as the number operator since \( |n\rangle \) is its eigenvector with eigenvalue \( n \),

\[
a^\dagger a|n\rangle = n|n\rangle.
\] (3.17)

The 2D Weyl equation (Eq. (3.8)) in a magnetic field becomes

\[
\hat{H}_W^s = \hbar v \mathbf{S} \cdot \mathbf{\Pi}
\]
\[= \hbar v (S_x \Pi_x + S_y \Pi_y)
\]
\[= \frac{\hbar v}{2} \left[ (S_x + iS_y)(\Pi_x - i\Pi_y) + (S_x - iS_y)(\Pi_x + i\Pi_y) \right]
\]
\[= \gamma (S_x a + S_y a^\dagger),
\] (3.18)

where \( \gamma = \hbar v / \sqrt{2} e B \) is an energy scale proportional to \( \sqrt{B} \). The continuous bands which exist under zero field (\( B = 0 \)) condense into discrete and highly degenerate LL’s, labelled
by integers \( n \). Written in matrix form, the Hamiltonian is

\[
\hat{H}_W^s = \gamma \begin{pmatrix}
0 & \rho_1 a \\
\rho_1 a^\dagger & 0 & \rho_2 a \\
& \ddots & \ddots & \ddots \\
& & 0 & \rho_{2s} a \\
& & & \rho_{2s} a^\dagger & 0
\end{pmatrix}.
\] (3.19)

From the symmetry of the Hamiltonian, it must be the case that the general form of the LL wavefunction is the spinor

\[
\psi_{\lambda,n} = \kappa (\alpha_1|n-2s\rangle, \alpha_2|n-2s+1\rangle, \ldots, \alpha_{2s+1}|n\rangle)^T,
\] (3.20)

where spinor elements are proportional to successive Fock states. To see this, if \( \psi \) is an energy eigenvector with eigenvalue \( \varepsilon \), its \( i \)th element must obey (from the Schrödinger equation)

\[
\varepsilon |\varphi_i\rangle = \rho_{i-1} a^\dagger |\varphi_{i-1}\rangle + \rho_i a |\varphi_{i+1}\rangle.
\] (3.21)

For \( |\varphi_i\rangle \propto |m\rangle \), this equality can only hold if \( |\varphi_{i-1}\rangle \propto |m-1\rangle \) and \( |\varphi_{i+1}\rangle \propto |m+1\rangle \).

The LL energies \( \varepsilon = \gamma \bar{\varepsilon} \) are obtained using the procedure of Lan, Goldman, Bermudez, Lu, and Öhberg in Ref. [17]. It involves the solution of a set of coupled linear equations to give a polynomial equation which is satisfied by the LL energy eigenvalues, \( \bar{\varepsilon} \). From the energy eigenequation \( \hat{H}\psi = \varepsilon \psi \), we obtain a set of \( 2s+1 \) coupled linear equations,

\[
\bar{\varepsilon} \alpha_1 = \sqrt{n-2s+1} \rho_1 \alpha_2;
\]

\[
\bar{\varepsilon} \alpha_m = \sqrt{n-2s+(m-1)\rho_{m-1} \alpha_{m-1} + \sqrt{n-2s+m\rho_m \alpha_{m+1}}}, \quad 1 < m < 2s;
\]

\[
\bar{\varepsilon} \alpha_{2s+1} = \sqrt{n \rho_{2s} \alpha_{2s}}.
\] (3.22)

The first in the set is an equation for the element \( \alpha_1 \) with a prefactor \( A_1 = \bar{\varepsilon} \). Multiplying the second equation by this prefactor, we can then eliminate \( A_1 \alpha_1 \) from it by substitution of the first equation. Collecting all the terms proportional to \( \alpha_2 \), the second equation now
Table 3.1: Expressions for the first few $A_m$ defined recursively in Eq. (3.25) which are used in building the Weyl Landau level energies for general pseudospin-$s$.

\begin{align*}
A_0 &= 1 \\
A_1 &= \bar{\epsilon} \\
A_2 &= \bar{\epsilon}^2 - (n - 2s + 1)\rho_1^2 \\
A_3 &= \bar{\epsilon}[\bar{\epsilon}^2 - (n - 2s + 1)\rho_1^2 - (n - 2s + 2)\rho_2^2] \\
A_4 &= \bar{\epsilon}^2[\bar{\epsilon}^2 - (n - 2s + 1)\rho_1^2 - (n - 2s + 2)\rho_2^2 - (n - 2s + 3)\rho_3^2] \\
&\quad - (n - 2s + 1)(n - 2s + 3)\rho_1^2\rho_3^2 \\
A_5 &= \bar{\epsilon}\left\{[\bar{\epsilon}^2 - (n - 2s + 4)\rho_1^2][\bar{\epsilon}^2 - (n - 2s + 1)\rho_1^2 - (n - 2s + 2)\rho_2^2] - \bar{\epsilon}^2(n - 2s + 3)\rho_3^2 \\
&\quad - (n - 2s + 1)(n - 2s + 3)\rho_1^2\rho_3^2\right\} \\
\end{align*}

reads

\[
\bar{\epsilon}A_1\alpha_2 = \sqrt{n - 2s + 1}\rho_1 A_1 \alpha_1 + \sqrt{n - 2s + 2}\rho_2 A_1 \alpha_3 \\
[\bar{\epsilon}A_1 - (n - 2s + 1)\rho_1^2]\alpha_2 = \sqrt{n - 2s + 2}\rho_2 A_1 \alpha_3. 
\] (3.23)

Now $\alpha_2$ has been isolated with the prefactor $A_2 = \bar{\epsilon}A_1 - (n - 2s + 1)\rho_1^2$. Multiplying the next equation by $A_2$ allows for the elimination of $A_2\alpha_2$, resulting in an equation which isolates $\alpha_3$ in terms of $\alpha_4$. Continuing in this way, we obtain

\[
A_m \alpha_m = \sqrt{n - 2s + m}\rho_m A_{m-1} \alpha_{m+1}, 
\] (3.24)

with

\[
A_0 = 1, \quad A_1 = \bar{\epsilon}, \quad A_m = \bar{\epsilon}A_{m-1} - (n - 2s + m - 1)\rho_{m-1}^2 A_{m-2}. 
\] (3.25)

Explicit expressions for $A_m$ up to $m = 5$ are provided in Table 3.1.

Ultimately, we arrive at the expression

\[
A_{2s+1} \alpha_{2s+1} = 0. 
\] (3.26)

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In no case can $\alpha_{2s+1}$ be zero. To see this, for any $\bar{\varepsilon}$, plugging $\alpha_{2s+1} = 0$ into Eq. (3.22) creates a cascade whereby every element is then zero, resulting in the the trivial vector (an unphysical wavefunction). Thus, Eq. (3.26) requires that

$$A_{2s+1} = 0.$$  \hspace{1cm} (3.27)

The condition in Eq. (3.27) creates a $(2s+1)$-order polynomial on $\bar{\varepsilon}$ whose set of solutions gives the energy eigenvalues at each $n$ (plotted in Fig. 3.2). For a given value of $n > 2s$, there will be $2s + 1$ different LL’s with energy $\bar{\varepsilon}_{\lambda,n}$. In a magnetic field, the numbers $\lambda = \{-s, ..., s\}$ are no longer band labels but rather label the branches off of which the LL’s bud. In the limit of zero field, then the set of $\lambda$ become the corresponding band labels and good quantum numbers again.

For odd values of $m$, $A_m$ is proportional to $\bar{\varepsilon}$. This means that for integer $s$, the condition $A_{2s+1} = 0$ puts an entire branch of LL’s ($\lambda = 0$) at exactly zero energy for all allowed $n$. The LL energies for pseudospin values up to $s = 2$ are presented in Table 3.2 and plotted in Fig. 3.2. The table is a reproduction of one from Ref. [17].

At low $n$ some of the branches have a reduced state space. For example, the $\lambda = 0$ branch in the $s = 2$ system is host to LL’s for all values of $n$ except for $n = 1$ and $n = 3$. The general form of the wavefunction in Eq. (3.20) shows that for $n < 2s$ the first $2s - n$ elements are exactly zero. As such, the Hilbert space is restricted and it is only possible here to construct $n + 1$ orthogonal wavefunctions. The pattern for the restricted state space in the flat branch (odd $n$ below $n = 2s$), and for the emergence of each finite-energy branch, can be argued in terms of particle-hole symmetry.

Consider first an integer-$s$ system. For the purposes of this discussion, assume that the region of $n < 2s$ is somewhat large. At $n = 0$, the Hilbert space is restricted such that only one LL can exist. Because the Weyl Hamiltonian is particle-hole symmetric (even in the presence of a magnetic field), this single LL must be at zero energy. Next, at $n = 1$ two LL’s exist which start the branches labelled $\lambda = \pm s$, with no level at zero energy. These branches have equal and opposite energy, adhering to the particle-hole symmetry. Further, at $n = 2$ an odd number of states exist and so the flat branch is again populated with a LL.
Figure 3.2: Weyl LL energies for various pseudospin-$s$ DW systems. The chemical potential $\mu = 0^+$ is illustrated with a green horizontal line, marking the divide between fully occupied (blue) and unoccupied (red) levels. Branches off of which the LL’s bud (dashed lines) are labelled from the bottom up with $\lambda = \{-s, ..., s\}$ as in Fig. 3.1.
Table 3.2: Landau level energies in the pseudospin-$s$ Weyl system up to $s = 2$. This table is a reproduction from Ref. [17].

<table>
<thead>
<tr>
<th>$s$</th>
<th>$\tilde{\varepsilon}_{\lambda,n}$</th>
<th>State Space</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2}$</td>
<td>$\tilde{\varepsilon}_{\pm \frac{1}{2},n} = \pm \sqrt{n}$</td>
<td>$n \geq 0$</td>
</tr>
<tr>
<td>1</td>
<td>$\tilde{\varepsilon}_{0,n} = 0$</td>
<td>$(n \geq 0) \cup (n \neq 1)$</td>
</tr>
<tr>
<td></td>
<td>$\tilde{\varepsilon}_{\pm 1,n} = \pm \sqrt{2(2n-1)}$</td>
<td>$n \geq 1$</td>
</tr>
<tr>
<td>$\frac{3}{2}$</td>
<td>$\tilde{\varepsilon}_{\pm \frac{3}{2},n} = \pm \sqrt{5(n-1) - \sqrt{16(n-1)^2 + 9}}$</td>
<td>$n \geq 2$</td>
</tr>
<tr>
<td></td>
<td>$\tilde{\varepsilon}_{\pm 3/2,n} = \pm \sqrt{5(n-1) + \sqrt{16(n-1)^2 + 9}}$</td>
<td>$n \geq 0$</td>
</tr>
<tr>
<td>2</td>
<td>$\tilde{\varepsilon}_{0,n} = 0$</td>
<td>$(n \geq 0) \cup (n \neq 1) \cup (n \neq 3)$</td>
</tr>
<tr>
<td></td>
<td>$\tilde{\varepsilon}_{\pm 1,n} = \pm \sqrt{5(2n-3) - 3 \sqrt{4n^2 - 12n + 17}}$</td>
<td>$n \geq 3$</td>
</tr>
<tr>
<td></td>
<td>$\tilde{\varepsilon}_{\pm 2,n} = \pm \sqrt{5(2n-3) + 3 \sqrt{4n^2 - 12n + 17}}$</td>
<td>$n \geq 1$</td>
</tr>
</tbody>
</table>

At $n = 3$, the next finite-energy branches emerge with labels $\lambda = \pm (s-1)$ and again there is no zero-energy level. In this way, all even values of $n < 2s$ have a zero-energy LL and $n$ finite-energy LL’s, while at odd-valued $n < 2s$ there is no zero-energy LL and one sees the emergence of the $m^{th}$ pair of finite-energy branches (where $m = (n + 1)/2$) counting from $|\lambda| = s$ pair inward to $|\lambda| = 1$.

Now consider the same construction, but with a half-integer-$s$ system. For the even $n < 2s$, where there is an odd number of LL’s, one of these LL’s must exist at zero energy. However, there is no zero-energy branch. Instead, each zero-energy LL at even $n < 2s$ is the emergence of the $m^{th}$ pair of branches counting down from $|\lambda| = s$, where now $m = (n/2)+1$. This single LL is shared between two equal-energy branches and is thus given the ambiguous label $\lambda = \tilde{0}$. The special zero-energy level in the $s = 1/2$ system, $\psi_{0,0}$, is responsible for anomalous effects seen in the graphene Hall and magneto-optical conductivities [3,13,51].

The wavefunction in Eq. (3.20) has a normalization factor $\kappa$, which allows for the freedom to choose the value of any one $\alpha_m$. From Eq. (3.24),

$$A_{2s} \alpha_{2s} = \sqrt{n} \rho_{2s} A_{2s-1} \alpha_{2s+1},$$  \hspace{1cm} (3.28)

choosing $\alpha_{2s+1} = A_{2s}$ then makes $\alpha_{2s} = \sqrt{n} \rho_{2s} A_{2s-1}$. Proceeding through decreasing values
Table 3.3: Landau level wavefunctions in the pseudospin-$s$ Weyl system up to $s = 2$. $\kappa$ is a normalization factor, different for each vector. These are the eigenvectors associated with the energy eigenvalues in Table 3.2. Some $n$ are not allowed for certain wavefunctions, outlined in Table 3.2.

<table>
<thead>
<tr>
<th>$s$</th>
<th>$\psi_{\lambda,n}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2}$</td>
<td>$\psi_{0,0} = (0,</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm\frac{1}{2},n \geq 1} = \kappa(</td>
</tr>
<tr>
<td>$1$</td>
<td>$\psi_{0,n} = \kappa(-\sqrt{n}</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm 1,n} = \kappa(\sqrt{n-1}</td>
</tr>
<tr>
<td>$\frac{3}{2}$</td>
<td>$\psi_{0,0} = (0, 0, 0,</td>
</tr>
<tr>
<td></td>
<td>$\psi_{0,2} = (0, -\sqrt{3n}</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm\frac{3}{2},n \geq 3} = \kappa(6\sqrt{n(n-1)(n-2)</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm\frac{3}{2},n \geq 1} = \kappa(6\sqrt{n(n-1)(n-2)</td>
</tr>
<tr>
<td>$2$</td>
<td>$\psi_{0,n} = \kappa(\sqrt{3(n-2)</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm 1,n} = \kappa(12\sqrt{n(n-1)(n-2)</td>
</tr>
<tr>
<td></td>
<td>$\psi_{\pm 2,n} = \kappa(12\sqrt{n(n-1)(n-2)</td>
</tr>
</tbody>
</table>
of $m$ in Eq. (3.24) with this choice leads to

$$\alpha_m = \left( \prod_{r=m}^{2s} \rho_r \sqrt{n-2s+r} \right) A_{m-1}. \quad (3.29)$$

This procedure only works if $\bar{\epsilon} \neq 0$. If instead $\bar{\epsilon} = 0$, then too many of the $A_m$'s are zero for Eq. (3.24) to be useful.

If instead $\bar{\epsilon} = 0$, then Eq. (3.22) rearranges to give the relationship

$$\alpha_m = \begin{cases} -\sqrt{\frac{n-2s+m+1}{n-2s+1}} \frac{\rho_{m+1}}{\rho_m} \alpha_{m+2} & \text{if } (2s+1-m) \text{ even} \\ 0 & \text{otherwise} \end{cases}. \quad (3.30)$$

The condition $(2s + 1 - m)$ being even means that $2s + 1$ is of the same character as $m$, either even or odd. Choosing a value of $\alpha_{2s+1} = 1$ leads to expressions for the other non-zero elements. For $2s + 1$ even,

$$\alpha_{2m} = (-1)^{s+m+\frac{1}{2}} \prod_{r=m}^{s-\frac{1}{2}} \sqrt{\frac{n-2s+2r+1}{n-2s+2r}} \frac{\rho_{2r+1}}{\rho_{2r}}, \quad m = 1, ..., s - \frac{1}{2}, \quad (3.31)$$

and for $2s + 1$ odd,

$$\alpha_{2m+1} = (-1)^{s+m} \prod_{r=m}^{s-1} \sqrt{\frac{n-2s+2r+2}{n-2s+2r+1}} \frac{\rho_{2r+2}}{\rho_{2r+1}}, \quad m = 0, ..., s - 1. \quad (3.32)$$

Expressions for the Weyl LL wavefunctions, constructed using Eqs. (3.29)-(3.32), are listed in Table 3.3 for pseudospin up to $s = 2$. The expressions for the $\lambda = 0$ wavefunctions in the $s = 1$ and $s = 2$ systems in Table 3.3 show that odd values of $n < 2s$ yield the trivial vector, making manifest the restrictions on the flat-branch state spaces given in Table 3.2.

### 3.3 Berry’s Phase in the Weyl System

Consider an adiabatic process on a wavefunction in which a continuous parameter (such as position, momentum, or magnetic field) is slowly varied before returning to its initial value. In addition to a dynamic phase (which will depend on the time spent on the path), the
wavefunction may acquire a nontrivial geometric phase should this path enclose a topological feature in parameter space, such as a Dirac point (Fig. 3.1). In recognition of his analysis in 1984, this measure of topology is referred to as Berry’s geometric phase [52].

A well known example is in the Aharanov-Bohm effect (ABE) [53]. A thin solenoid produces an axis of magnetic flux which represents a topological defect in real space. Should an electron take two paths around the solenoid and rejoin, a non-zero phase is acquired which creates a measurable shift in interference patterns. The Berry phase also plays an important role in the theory of the integer quantum Hall effect (QHE) by Thouless, Kohmoto, Nighingale, and den Nijs [54]. In the QHE, the Hall conductivity of a 2D electron gas is an integer multiple of the magnetic flux quantum, \( \sigma_H = \nu e^2 / h \). According to Thouless et al., each filled LL in the system provides exactly one quantum of flux to the conductivity as a result of the non-zero Berry phase associated with each LL. As such, \( \nu \) is a measure of the number of filled LL’s in the electron gas. Of course, these theories for both the ABE (1959) and QHE (1982) were arrived at before Berry’s important discussion of the geometric phase (1984).

In a Dirac-Weyl system, each band is assigned a Berry phase associated with a path \( C \) that encloses the Dirac point in reciprocal space. This is different from the ABE or QHE in that the topological defect is an integral part of the system and not provided via a solenoid or induced via an external magnetic field. It is well known that graphene, the pseudospin-1/2 system, exhibits Berry phases of \( \gamma_{\pm}(C) = \mp \pi \) for the upper and lower cones, respectively [3]. In this section the Berry phase is derived for the general pseudospin-\( s \) Weyl systems. This was essentially done by Berry, but in the context of the interaction between a magnetic quantum spin and a magnetic field [52]. Such an interaction is described by the Weyl Hamiltonian (Eq. 3.8), but with momentum \( \mathbf{k} \) replaced by magnetic field \( \mathbf{B} \) and with \( v \) replaced by a factor involving the gyromagnetic ratio. In this section, greek labels placed on vectors and tensors, \( x^\mu \), refer to spatial indices only (i.e., \( \mu \neq 0 \)). Inner products \( x^\mu y_\mu \) are the straight-forward Euclidean dot product.

Consider a multi-band (or multi-level) system where a state in band \( a \) is labelled by the set of parameters \( \mathbf{k} (|a(\mathbf{k})\rangle) \). As \( \mathbf{k} \) is slowly varied along a closed path \( C \), the state function
acquires a geometric phase (in addition to the dynamic one),

\[ \tilde{\gamma}_\alpha(C) = \oint_C dk^\mu A_\mu, \tag{3.33} \]

where

\[ A_\mu(a(k)) = i\langle a(k)|\partial_\mu a(k)\rangle, \quad \partial_\mu \equiv \frac{\partial}{\partial k^\mu}, \tag{3.34} \]

is referred to as the Berry connection. Note that \( \langle a|\partial_\mu a \rangle \) is purely imaginary. To see this, take the derivative of the orthonormality relation \( \langle a|a \rangle = 1, \)

\[ \langle \partial_\mu a|a \rangle + \langle a|\partial_\mu a \rangle = 0 \quad \Rightarrow \quad \langle a|\partial_\mu a \rangle = -\left( \langle a|\partial_\mu a \rangle \right)^*, \tag{3.35} \]

proving that \( \langle a|\partial_\mu a \rangle \) is in fact imaginary. As such, the Berry connection can be written

\[ A_\mu = -\text{Im} \langle a|\partial_\mu a \rangle. \tag{3.36} \]

\( A_\mu \) is not invariant to a choice of the \( U(1) \) gauge on the state. Consider, for example, the same physical state under a different gauge, \( |b\rangle = e^{i\alpha}|a\rangle \), where \( \alpha \) can depend on \( k \) in general. Then

\[ \langle b|\partial_\mu a \rangle = \langle a|\partial_\mu a \rangle + i\partial_\mu \alpha. \tag{3.37} \]

Based on Eq. (3.37), we can view \( A_\mu \) as a vector potential in reciprocal space which is only unique up to some gradient term \( \partial_\mu \alpha \). This prompts the definition of a gauge-invariant field strength,

\[ F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \]

\[ = -\text{Im} \left( \langle \partial_\mu a|\partial_\nu a \rangle - \text{c.c.} \right) \tag{3.38} \]

\[ = -2\text{Im} \langle \partial_\mu a|\partial_\nu a \rangle, \]

where ‘c.c.’ stands for complex conjugate. \( F_{\mu\nu} \) is referred to as the Berry curvature, which can be pieced out of the integrand of Eq. (3.33) via Stokes’ theorem. This now gives a
unique definition of the Berry phase,

$$\gamma_a(C) = \frac{1}{2} \int_{\Sigma} d\sigma^{\mu\nu} F_{\mu\nu} ,$$  \hspace{1cm} (3.39)

where $\Sigma$ is the surface enclosed by $C$ which has an infinitesimal unit of area $d\sigma^{\mu\nu}$.

The Berry curvature in Eq. (3.38) can be taken further by first inserting the resolution of the identity, $1 = \sum_b |b\rangle\langle b|,$

$$F_{\mu\nu} = -2\text{Im} \sum_{a \neq b} \langle \partial_\mu a | b \rangle \langle b | \partial_\nu a \rangle.$$  \hspace{1cm} (3.40)

The $a = b$ term is not included since $\langle \partial_\mu a | a \rangle$ and $\langle a | \partial_\nu a \rangle$ are both imaginary, making their product entirely real. To move the derivative operator off of the state function, we consider the stationary Schrödinger equation, $\hat{H}|a\rangle = \varepsilon_a |a\rangle$. Schrödinger implies

$$\partial_\mu (\hat{H}|a\rangle) = \partial_\mu (\varepsilon_a |a\rangle)$$

$$\partial_\mu \hat{H}|a\rangle + \hat{H}|\partial_\mu a\rangle = \partial_\mu \varepsilon_a |a\rangle + \varepsilon_a |\partial_\mu a\rangle$$ \hspace{1cm} (3.41)

Acting on the left with $\langle b|$ gives

$$\langle b|(\hat{H} - \varepsilon_a)|\partial_\mu a\rangle = -\langle b|(\partial_\mu \hat{H} - \partial_\mu \varepsilon_a)|a\rangle$$

$$\langle \varepsilon_b - \varepsilon_a | \partial_\mu a \rangle = -\langle b|\partial_\mu \hat{H}|a\rangle + \partial_\mu \varepsilon_a \langle b|a\rangle$$ \hspace{1cm} (3.42)

$$\langle b|\partial_\mu a \rangle = \frac{\langle b|\partial_\mu \hat{H}|a\rangle}{\varepsilon_a - \varepsilon_b} , \text{ if } a \neq b .$$

Similarly,

$$\langle \partial_\mu a | b \rangle = \frac{\langle a|\partial_\mu \hat{H}|b\rangle}{\varepsilon_a - \varepsilon_b} , \text{ if } a \neq b .$$  \hspace{1cm} (3.43)

Then the Berry phase can be written

$$\gamma_a(C) = -\text{Im} \int_{\Sigma} d\sigma^{\mu\nu} \sum_{a \neq b} \frac{\langle a|\partial_\mu \hat{H}|b\rangle \langle b|\partial_\nu \hat{H}|a\rangle}{(\varepsilon_a - \varepsilon_b)^2} .$$  \hspace{1cm} (3.44)

By moving the derivative operator onto the Hamiltonian, this form of the Berry’s phase
works for wavefunctions that are not single-valued everywhere (like at the location of a Dirac point).

The denominator in the integrand of Eq. (3.44) shows that if two bands have the same energy at a single point covered by $\Sigma$, then this region will provide the dominant contribution to the integral. A theorem by von Neumann and Wigner states that no matter the size of a Hermitian matrix (such as the matrix form of a Hamiltonian), three parameters must be varied in order for a degeneracy to ‘accidentally’ occur [55]. This accidental occurrence refers to a single-point band touching that is not protected by any special symmetries of the matrix. Accordingly, in a DW system (where there are only two variable parameters $k_x$ and $k_y$) the degeneracy in the Dirac point is protected by additional symmetries. For example, the Dirac point in graphene is protected by time-reversal and inversion symmetries. If one of these symmetries were broken, a term proportional to $S^z$ appears in the Hamiltonian. Giving the symmetry breaking a strength of $\Delta$, the K-point graphene Hamiltonian becomes

$$\hat{H} = \hbar v (S^x k_x + S^y k_y) + \Delta S^z.$$  \hspace{1cm} (3.45)

The new energy eigenvalues are $\varepsilon_{\pm} = \pm \sqrt{\hbar^2 v^2 k^2 + \Delta^2}$. Thus, a gap equal to $2|\Delta|$ opens up at $k = 0$. This shows that the degeneracy point in graphene is protected by the existence of time-reversal and inversion symmetry. If $\Delta$, however, was a variable parameter of the system, then a degeneracy occurs at $k_x = k_y = \Delta = 0$.

In order to deal with graphene and the other 2D Weyl systems in calculating the Berry phase, we must allow for an isotropic extension into three dimensions. That is, use the 3D Weyl system, but assume that $C$ is restricted to the $k_x k_y$-plane. This way there are three parameters in the Hamiltonian to vary,

$$\hat{H} = \hbar v (S^x k_x + S^y k_y + S^z k_z).$$  \hspace{1cm} (3.46)

Should some symmetry-breaking perturbation $\Delta$ enter, this would only act to shift the degeneracy rather than open it. The singularity is totally protected. Working in 3D parameter
space, it is convenient to switch to the cross-product notation,

$$\gamma_a(C) = - \int_{\Sigma} d\mathbf{s} \cdot \mathbf{V}_a, \quad (3.47)$$

where $d\mathbf{s}$ is the normal vector to the infinitesimal area $d\sigma^\mu \nu$ and

$$\mathbf{V}_a = \text{Im} \sum_{a \neq b} \frac{\langle a | \partial \hat{H} | b \rangle \times \langle b | \partial \hat{H} | a \rangle}{(\varepsilon_a - \varepsilon_b)^2}. \quad (3.48)$$

The isotropy of the Weyl Hamiltonian can be exploited to easily determine the Berry curvature $\mathbf{V}_a$. At each fixed point $\mathbf{k}$, we construct a new set of coordinates $\mathbf{q}$ so that the $z$-direction of $\mathbf{q}$ points along $\mathbf{k}$. This way $\hat{H} = \hbar vq S_z$ and we can use the $S_z$ basis, where $|a = \{1, \ldots, 2s + 1\}\}$ is the $a^{th}$ eigenvector of $S_z$ with eigenvalue $\lambda = s + 1 - a$. In this convenient basis, the $m^{th}$ element of the vector $|a\rangle$ is $\delta_{a,m}$ (one element is equal to one and the rest zero). With $\partial \hat{H} = \hbar vS$, we make use of the matrix elements from Eq. (3.7),

$$\langle b | S^x | a \rangle = \frac{1}{2}(\rho_a \delta_{b,a+1} + \rho_b \delta_{a,b+1})$$
$$\langle b | S^y | a \rangle = \frac{1}{2}(\rho_a \delta_{b,a+1} - \rho_b \delta_{a,b+1}) \quad (3.49)$$
$$\langle b | S^z | a \rangle = (s + 1 - a)\delta_{a,b}.$$  

This shows that in these temporary coordinates, only the $z$-component of $\mathbf{V}_a$ is non-zero since the other components have terms proportional to $\langle b | S^z | a \rangle = 0$ (since $a \neq b$). Then the only expression required is

$$\langle a | S^x | b \rangle \langle b | S^y | a \rangle = \frac{i}{4}(\rho^2_a \delta_{b,a+1} - \rho^2_{a-1} \delta_{b,a-1}). \quad (3.50)$$

Based on this expression, the only contributions to the Berry phase in band $a$, $\gamma_a$, are from those bands adjacent to $a$, $b = a \pm 1$. The energy difference between adjacent bands at the
same momentum is $\varepsilon_{a+1} - \varepsilon_a = \hbar v k$. Then we obtain

$$V_{a,z} = \begin{cases} 
\frac{\rho_1^2}{2k^2} & \text{if } a = 1 \ (\lambda = s) \\
\frac{(\rho_a^2 - \rho_{a-1}^2)}{2k^2} & \text{if } 1 < a < 2s + 1 \ (-s < \lambda < s) \\
-\frac{\rho_2^2}{2k^2} & \text{if } a = 2s + 1 \ (\lambda = -s) 
\end{cases} \quad (3.51)$$

But, $\rho_1^2 = \rho_2^2 = 2s$ and

$$\rho_a^2 - \rho_{a-1}^2 = a(2s + 1 - a) - (a - 1)(2s + 2 - a)$$
$$= a(2s + 2 - a) - a - (a - 1)(2s + 2 - a)$$
$$= 2(s + 1 - a)$$
$$= 2\lambda. \quad (3.52)$$

The standard SU(2) label $\lambda = s + 1 - a$ has been recovered in each case of Eq. (3.51) and it will now be used in the place of the ordinal band index $a$.

In the temporary coordinates, where the $q_z$ has been placed in the direction of momentum,

$$V_{\lambda,x} = 0, \ V_{\lambda,y} = 0, \ V_{\lambda,z} = \frac{\lambda}{k^2}. \quad (3.53)$$

Rotating back to the original coordinate system, we obtain

$$V_{\lambda} = \frac{\lambda k}{k^3}. \quad (3.54)$$

Substituting this in for the integrand in Eq. (3.47) and focusing in on the singularity at $k = 0$,

$$\gamma_{\lambda}(C) = -\lambda \int_{\Sigma \to 0} \frac{ds \cdot k}{k^3} \quad (3.55)$$

This can be recognized as the formula for the flux through a surface $\Sigma$ (in reciprocal space) of a magnetic monopole located at $k = 0$ [35]. The result of the integral is the solid angle subtended by $C$ from the origin, $\Omega(C)$. With $C$ restricted to a 2D plane, $\Omega(C) = 2\pi$. Thus,
the gauge-invariant Berry phase for band $\lambda = \{-s, ..., s\}$ in the pseudospin-$s$ Weyl system is

$$\gamma_\lambda(C) = -2\pi \lambda.$$  

(3.56)

Adjacent bands are different in their Berry phase by steps of $2\pi$. For odd values of $2s+1$, the flat band has a Berry phase of zero and all cones have an even factor of $\pi$ as the Berry phase. For even-valued $2s+1$, $\gamma_\lambda(C)$ is an odd multiple of $\pi$ in each band. This means that a revolution around the Dirac point results in a factor of $-1$ on the wavefunction. A Berry phase of $\pm\pi$ was one of the first hallmark measurements identifying graphene as a pseudospin-1/2 Dirac-Weyl material [3].

### 3.4 The Dice Lattice and the $\alpha$-$T_3$ model

The tight-binding band structure of graphene was first calculated by Wallace in 1947 [4]. It was then Semenoff in 1984 who identified the low-energy dynamics in graphene as the pseudospin-1/2 Dirac-Weyl system [10]. In graphene, the two pseudospin projections, $\lambda = \pm 1/2$, refer to two sublattice degrees of freedom.

The hexagonal (or honeycomb) lattice made up of carbon atoms in graphene is illustrated in Fig. 3.3(a). In the figure, the A sites are coloured red and connected with a faint dashed line that shows the triangular sublattice. The B sublattice (in blue) is situated so that the B sites lie in the centre of alternating A-sublattice plaquettes. The carbon atoms are $sp^2$-hybridized, so that for each atom, three of the free electrons are localized in $\sigma$-bonds between adjacent atoms. The remaining free electron from the $p_z$ atomic orbital goes into a delocalized $\pi$-bond, becoming a conduction electron. These conduction electrons, one per carbon-atom site, make up the ‘electron soup,’ or quantum vacuum, which gives rise to relativistic quasiparticle excitations. A pseudospin-‘up’ quasiparticle ($\lambda = +1/2$) is a Bloch state associated with sublattice A, pseudospin-‘down’ ($\lambda = -1/2$) with sublattice B, and a superposition of spins has the quasiparticle smeared over both sublattices.

Starting from the graphene configuration, the dice lattice is constructed by introducing an additional triangular sublattice C, shifted relative to B in the same way that B is shifted relative to A. This C sublattice is then bonded to B sites only, assuming one free conduction
Figure 3.3: 2D (a) graphene and (b) dice lattices. The triangular sublattices are labelled A (red), B (blue), and C (green). In (a), the A sublattice is illustrated with a faint dashed line for clarity. Solid lines represent chemical bonds.

electron per site as in graphene. The dice lattice, also called the $T_3$ lattice because of its symmetries, is sketched in Fig. 3.3 with the C lattice coloured green. Like graphene, its low-energy dynamics are described by the DW Hamiltonian (Eq. (3.8)), but with a pseudospin of $s = 1$. With a third sublattice degree of freedom, this system has three projections in the low-energy quasiparticles, $\lambda = \{+1, 0, -1\}$, referring to sublattice A, B, and C, respectively.

While graphene exists in nature as a carbon allotrope, the dice lattice is hypothetical at this time. However, it is theoretically possible to construct a synthetic dice-lattice condensed matter system with photonic lattices or arrays of optically trapped ultra-cold atoms [19]. The dice lattice also offers a useful toy model for theorists studying the pseudospin-1 Dirac-Weyl system.

Dóra, Kailasvuori, and Moessner extend this blueprint by overlaying and bonding $2s + 1$ triangular sublattices to construct a hypothetical pseudospin-$s$ Dirac-Weyl system [18]. In this section, it is demonstrated in detail how a tight-binding Hamiltonian on one of these lattices can lead to a relativistic system at low energy. Because this calculation has been done for graphene in many places [4,10,13,39,56], it is instead presented here for the dice lattice.
The nearest-neighbour tight-binding Hamiltonian for the dice lattice is

\[ \hat{H} = t \sum_{\langle ij \rangle} c_i^\dagger c_j, \]  

(3.57)

where \( t \) is the hopping strength (assumed to be equal for each bond). \( c_i^\dagger \) and \( c_i \) are the electron creation and annihilation operators for site \( i \) and the summation is only taken over bonded sites \( \langle ij \rangle \) (nearest-neighbour hopping). These fermionic Fock operators obey an anticommutation relation,

\[ \{ c_i^\dagger, c_j \} = \delta_{i,j}. \]  

(3.58)

It is convenient to separate out individual operators for A, B, and C sites. We can then carry out a sum first over all B sites and then at each B site sum over the three A sites and C sites bonded to it. The Hamiltonian can be written in matrix form,

\[ \hat{H} = t \sum_{i=1}^{N} \sum_{j=1}^{3} \begin{pmatrix} c_{A,j}^\dagger & c_{B,i}^\dagger & c_{C,j}^\dagger \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_{A,j} \\ c_{B,i} \\ c_{C,j} \end{pmatrix}, \]  

(3.59)

where \( N \) is the number of B sites in the lattice.

Next a Fourier transform is made from direct to reciprocal space so that an operator is written

\[ c_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}}^{\text{BZ}} e^{-i\mathbf{k} \cdot \mathbf{x}_i} d_{\mathbf{k}}^\dagger, \]  

(3.60)

where the summation is taken over all wavevectors \( \mathbf{k} \) in the Brillouin zone (BZ), \( \mathbf{x}_i \) is the position of the \( i \)th site, and \( d_{\mathbf{k}}^\dagger \) is the momentum space creation operator conjugate to the annihilation operator \( d_{\mathbf{k}} \), such that

\[ \{ d_{\mathbf{k}}^\dagger, d_{\mathbf{q}} \} = \delta_{\mathbf{k},\mathbf{q}}. \]  

(3.61)

Then, using \( \mathbf{w}_{A,j} \) as the location of the \( j \)th A site relative to a B site, a typical term
transforms in the following way,
\[
\sum_{i=1}^{N} c_{A,j}^\dagger c_{B,i} = \frac{1}{N} \sum_{k,q} e^{-i[k(x_{B,i}+w_{A,j}) - q_x x_{B,i}]} d_{A,k}^\dagger d_{B,q}
\]
\[
= \sum_{k,q} \left( \frac{1}{N} \sum_{i=1}^{N} e^{-i x_{B,i} (k - q)} \right) e^{-i k \cdot w_{A,j}} d_{A,k}^\dagger d_{B,q}
\]
\[
= \sum_{k,q} \delta_{k,q} e^{-i k \cdot w_{A,j}} d_{A,k}^\dagger d_{B,q}
\]
\[
= \sum_{k} e^{-i k \cdot w_{A,j}} d_{A,k}^\dagger d_{B,k}.
\]

The piece in the large round brackets on the second line of Eq. (3.62) is a generalized form equivalent to the Kronecker delta, \( \delta_{k,q} \). After the Fourier transform, each term in the Hamiltonian is diagonal in \( k \). The Hamiltonian becomes

\[
\hat{H} = t \sum_{k} \sum_{j=1}^{3} \begin{pmatrix} d_{A,k}^\dagger & d_{B,k}^\dagger & d_{C,k}^\dagger \end{pmatrix} \begin{pmatrix} 0 & e^{-i k \cdot w_{A,j}} & 0 \\ e^{i k \cdot w_{A,j}} & 0 & e^{i k \cdot w_{B,j}} \\ 0 & e^{-i k \cdot w_{B,j}} & 0 \end{pmatrix} \begin{pmatrix} d_{A,k} \\ d_{B,k} \\ d_{C,k} \end{pmatrix}.
\]

(3.63)

Based on the orientation in Fig. 3.3(a) and using a bond length of \( a \), the six separation vectors from the hub (blue B sites in the figure) are

\[
w_{A,1} = (0, a), \quad w_{A,2} = \left( \frac{\sqrt{3} a}{2}, -\frac{a}{2} \right), \quad w_{A,3} = \left( -\frac{\sqrt{3} a}{2}, -\frac{a}{2} \right),
\]
\[
w_{B,1} = (0, a), \quad w_{B,2} = \left( \frac{\sqrt{3} a}{2}, \frac{a}{2} \right), \quad w_{B,3} = \left( -\frac{\sqrt{3} a}{2}, \frac{a}{2} \right).
\]

(3.64)

Then, on the full energy scale of the charge-carriers (spanning a range of \( 6\sqrt{2}t \)), the single-particle Hamiltonian is

\[
\hat{H}(k) = \begin{pmatrix} 0 & tf(k) & 0 \\ tf^\ast(k) & 0 & tf(k) \\ 0 & tf^\ast(k) & 0 \end{pmatrix},
\]

(3.65)

where

\[
f(k) = e^{-i k_y} + 2e^{-\frac{\sqrt{3}}{2} k_y} \cos \left( \frac{\sqrt{3} a}{2} k_x \right).
\]

(3.66)
Diagonalizing Eq. (3.65) gives the three energy bands in the dice lattice,

\[\varepsilon_0(k) = 0,\]

\[\varepsilon_{\pm 1}(k) = \pm \sqrt{2|t|f} = \pm t \sqrt{2 \left[ 3 + 2 \cos(\sqrt{3} ak_x) + 4 \cos \left( \frac{3a}{2} k_y \right) \cos \left( \frac{\sqrt{3}a}{2} k_x \right) \right]} \quad (3.67)\]

The full dice lattice band structure is plotted in Fig. 3.4 which assumes a two-thirds filling so that the flat band and negative-energy bands are filled (blue) and the positive-energy band is empty (red). The hexagonal Brillouin zone (BZ) is traced out in black, showing band-touching points at its six vertices.

It can be shown that the element of the \( \lambda = 0 \) wavefunction associated with sublattice B is always zero. This means that the hub sites in Fig. 3.3(b) can not be traversed by nearest-neighbour-hopping electrons (Eq. (3.57)). Flat-band electrons are localized to rim sites (sublattices A and C), so that they have no dynamics and hence zero energy.

The BZ has a total of two inequivalent band-touching points located at

\[\mathbf{K} = \left( -\frac{4\pi}{3\sqrt{3}a}, 0 \right), \quad \mathbf{K}' = \left( \frac{4\pi}{3\sqrt{3}a}, 0 \right) \quad (3.68)\]

The regions around these two \( \mathbf{K} \) points are referred to as valleys in the band structure. Expanding \( f \) in small values of \( \mathbf{k} \) about these two points gives

\[f|_{\mathbf{K}} \approx \frac{3a}{2} k_-, \quad f|_{\mathbf{K}'} \approx -\frac{3a}{2} k_+, \quad (3.69)\]

where \( k_\pm = k_x \pm ik_y \). Then the low-energy Hamiltonian about the K-point is

\[\hat{\mathcal{H}} = \frac{3at}{2} \begin{pmatrix} 0 & k_- & 0 \\ k_+ & 0 & k_- \\ 0 & k_+ & 0 \end{pmatrix} = \hbar v S_1 \cdot \mathbf{k}, \quad (3.70)\]

where \( v = \frac{3at}{\sqrt{2}\hbar} \) and \( S_1 \) are the spin-1 matrices. Thus, the low energy dynamics around the K-point are described by the pseudospin-1 right-handed Dirac-Weyl equation (Eq. (3.8)). The \( \mathbf{K}' \)-point, with \( S_1 \to -S_1^* \), is host to left-handed Dirac-Weyl fermions. Since the dice
Figure 3.4: Nearest-neighbour tight-binding band structure for the dice lattice in Fig. 3.3(b) using Eq. (3.67). A two-thirds filling is illustrated so that the negative-energy and flat bands are occupied (blue) and the positive-energy band unoccupied (red). The hexagonal BZ is traced out in black.
lattice at low energy is described by two independent $3 \times 3$ sectors, the full low-energy Hamiltonian is a $6 \times 6$ block-diagonal object,

$$
\hat{H}_{\text{dice}} = \begin{pmatrix}
\hat{H}_{W,r}^{1} & 0 \\
0 & \hat{H}_{W,\ell}^{1}
\end{pmatrix}.
$$

(3.71)

The distinct chirality $(r, \ell)$ between the two sectors does not have any bearing on certain observables. For many physical quantities, such as conductivity or polarizability, it is sufficient to simply use only one of the chiral centres to describe the dice lattice and simply include a factor of two to account for the two-fold valley degeneracy.

An interesting variant to the dice lattice is in the $\alpha$-T$_3$ model [22, 23]. Starting with graphene in Fig. 3.3(a), the third triangular sublattice is bonded not with the same hopping strength $t$ as in Fig. 3.3(b), but instead is given a variable hopping parameter $\alpha t$, where $\alpha \in [0, 1]$. The unit cell for $\alpha$-T$_3$, centred around the C site, is illustrated in Fig. 3.5. The A and B sublattice sites (red and blue, respectively) are bonded with a fixed hopping parameter $t$. The C site (green) is bonded only to the B sites with a hopping parameter that can vary continuously from 0 to $t$. At $\alpha = 1$, the dice lattice in Fig. 3.3(b) is recovered. For $\alpha = 0$, one is left with the graphene lattice in Fig. 3.3(a) but with an additional inert triangular sublattice which does not contribute to any dynamics in the system.

Like graphene and the dice lattice, the $\alpha$-T$_3$ model is host to two independent band-touching points, K and K'. Around the K-point, the low-energy Hamiltonian is

$$
\hat{H}_\alpha = \frac{\hbar v}{\sqrt{1 + \alpha^2}} \begin{pmatrix}
0 & k_- & 0 \\
k_+ & 0 & ak_- \\
0 & ak_+ & 0
\end{pmatrix} = \frac{2(1 - \alpha)}{\sqrt{1 + \alpha^2}} (\hat{H}_{W}^{1/2} \oplus \emptyset) + \frac{\sqrt{2\alpha}}{\sqrt{1 + \alpha^2}} \hat{H}_{W}^{1},
$$

(3.72)

where $\emptyset$ represents the inert C sublattice when $\alpha = 0$. Equation (3.72) separates out the pseudospin-1/2 and pseudospin-1 parts of the Hamiltonian. This shows that a quasiparticle excitation in the $\alpha$-T$_3$ model at an intermediate value of $\alpha$ is a hybrid pseudospin-1 and pseudospin-1/2 Dirac-Weyl fermion [24].

No matter the value of $\alpha$, the energy dispersion from Eq. (3.72) is the same as the $s = 1$
Figure 3.5: Unit cell for the α-$T_3$ model. A (red) and B (blue) sublattice sites are bonded with hopping strength $t$, the C (green) site is bonded to the B sites with a variable hopping strength $\alpha t$, $\alpha \in [0,1]$.

Weyl system in Fig. 3.1. However, the variability of $\alpha$ does affect other properties, such as the Berry phase,

\[
\tilde{\gamma}_\pm(C) = \pi(1 - \alpha^2)/(1 + \alpha^2),
\]
\[
\tilde{\gamma}_0(C) = 2\pi(\alpha^2 - 1)/(1 + \alpha^2),
\]

for the cones and flat band, respectively [22]. Note that these are not the gauge-invariant Berry phases, $\gamma_\alpha(C)$, discussed in the previous section, but they still demonstrate a variability based on $\alpha$. That the Berry phase is allowed to vary continuously with $\alpha$ means that it is not a topological property in the $\alpha$-$T_3$ system.

3.5 MCT and the Kane Model

The zincblende diatomic lattice structure (Fig. 3.6) is a 3D array in which two different atoms alternate on tetrahedral centres. In 1957, Kane calculated the band structure of the
zincblende semiconductor InSb using a method that deals with the material’s small band gap [32]. Today, the Kane model is broadly used for various zincblende structures, including Hg$_{1-x}$Cd$_x$Te (MCT) [24,29].

At low energy, up to linear order in momentum, the Kane model Hamiltonian reads

$$\hat{H}_{\text{Kane}} = \hbar v$$

where

$$\begin{pmatrix}
0 & \sqrt{k_\perp} & 0 & 0 & 0 & 0 & 0 & 0 \\
\sqrt{3}k_\perp & \frac{E_g}{\hbar v} & -k_\perp & -\frac{k_z}{\sqrt{2}} & -\frac{k_z}{\sqrt{2}} & -k_z & 0 & 0 \\
0 & -k_\perp & 0 & 0 & 0 & 0 & -k_z & 0 \\
0 & -\frac{k_z}{\sqrt{2}} & 0 & -\frac{\Delta}{\hbar v} & 0 & 0 & -\frac{k_z}{\sqrt{2}} & 0 \\
0 & -\frac{k_z}{\sqrt{2}} & 0 & 0 & -\frac{\Delta}{\hbar v} & 0 & -\frac{k_z}{\sqrt{2}} & 0 \\
0 & -k_z & 0 & 0 & 0 & 0 & k_\perp & 0 \\
0 & 0 & -k_z & -\frac{k_z}{\sqrt{2}} & -\frac{k_z}{\sqrt{2}} & -k_z & \frac{E_g}{\hbar v} & -\frac{\sqrt{3}k_\perp}{2} \\
0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}k_\perp}{2} & 0 \\
\end{pmatrix}$$

$$E_g$$ is a small band gap parameter and $$\Delta$$ is a large one. This $8 \times 8$ Hamiltonian gives rise to four doubly degenerate bands, which are plotted in Fig. 3.7 for three different
Figure 3.7: Kane model band structure for zero magnetic field with parameters $v = 1.06 \times 10^6 \text{ m/s}$, $E_g = 4 \text{ meV}$, and (a) $\Delta \rightarrow \infty$, (b) $\Delta = 1 \text{ eV}$, and (c) $\Delta = 0.4 \text{ eV}$.

values of $\Delta$. The parameters $v = 1.06 \text{ m/s}$, $E_g = 4 \text{ meV}$, and $\Delta = 1 \text{ eV}$ (Fig. 3.7(b)) are applicable to MCT with a critical Cd:Te ratio $x = x_c \approx 0.17 \ [29]$. A three-quarters filling also applies to neutral MCT, leaving the top band unoccupied.

The band structure in Fig. 3.7 shows that the top three bands resemble the pseudospin-1 Weyl dispersion in Fig. 3.1. Two conic bands are separated by a small gap $E_g$ (indiscernible on the scale in Fig. 3.7). The extended Kane model (higher-order in momentum) contains a heavy hole band with very broad curvature, but at linear order in momentum this nominally flat band is at exactly zero energy. A fourth band is located below the rest, separated by the large gap $\Delta$. The figure shows that as $\Delta$ is decreased, the approach of this fourth band to the others induces some curvature in the conic bands.

In general, the energy dispersion extracted from Eq. (3.74) cannot be solved analytically (except for the flat band with energy $\varepsilon = 0$). However, taking $\Delta \rightarrow \infty$ decouples the fourth and fifth columns of the matrix in Eq. (3.74), effectively removing the fourth band from the picture. This leads to a simpler and more tractable Hamiltonian, but one which does not
describe MCT as accurately. This reduced $6 \times 6$ Hamiltonian is

$$\hat{\mathcal{H}}_{\text{Kane}} = \begin{pmatrix}
\hat{\mathcal{H}}_A & hvk_z \hat{C} \\
0 & \hat{\mathcal{H}}_B
\end{pmatrix},$$

(3.75)

where the two 2D sectors labelled A and B,

$$\hat{\mathcal{H}}_A = hv \begin{pmatrix}
0 & \frac{\sqrt{3}k_-}{2} & 0 \\
\frac{\sqrt{3}k_+}{2} & \frac{E_g}{nv} & -\frac{k_+}{2} \\
0 & -\frac{k_+}{2} & 0
\end{pmatrix}, \quad \hat{\mathcal{H}}_B = hv \begin{pmatrix}
0 & k_- \frac{1}{2} & 0 \\
k_+ \frac{1}{2} & \frac{E_g}{nv} & -\frac{\sqrt{3}k_-}{2} \\
0 & -\frac{\sqrt{3}k_+}{2} & 0
\end{pmatrix},$$

(3.76)

are connected by the third dimension $k_z$ via the matrix

$$\hat{C} = \begin{pmatrix}
0 & 0 & 0 \\
-1 & 0 & 0 \\
0 & -1 & 0
\end{pmatrix}.$$  

(3.77)

The Hamiltonian in Eq. (3.75) can be solved, giving the three energy bands labelled $\lambda = \{0, \xi = \pm 1\}$,

$$\varepsilon_0(k) = 0, \quad \varepsilon_\xi(k) = \left(E_g/2\right) + \xi \sqrt{\left(E_g/2\right) + (hv)^2}.$$  

(3.78)

This dispersion is illustrated in Fig. 3.8 for various $E_g$, demonstrating the transition from semiconductor ($E_g > 0$) to semimetal ($E_g < 0$). At $E_g = 0$, the cones linearize and touch at a single point intersecting the flat band.

If one were to restrict the system to two dimensions by setting $k_z = 0$, the Kane Hamilton becomes block diagonal,

$$\hat{\mathcal{H}}^{2\text{D}}_{\text{Kane}} = \hat{\mathcal{H}}_A \oplus \hat{\mathcal{H}}_B.$$  

(3.79)

Comparison to Eq. (3.72) shows that $\hat{\mathcal{H}}_A$ in Eq. (3.76) maps onto the K-point Hamiltonian in the $\alpha-T_3$ model with the value $\alpha = -1/\sqrt{3}$. The same value maps $\hat{\mathcal{H}}_B$ onto the K’ point. While the $\alpha-T_3$ model was constructed with $\alpha \in [0, 1]$ in mind, it is fine to extend this range to $\alpha \in [-1, 1]$ because of the duality $\alpha \leftrightarrow -\alpha$. This duality exists because the sign on $\alpha$ in the $\alpha-T_3$ Hamiltonian (Eq. (3.72)) can be flipped using the transformation $\hat{\mathcal{H}} \rightarrow \hat{U} \hat{\mathcal{H}} \hat{U}^T$. 

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Figure 3.8: Band structure of the reduced Kane model showing an evolution through tuning of the gap $E_g$.

with $\hat{U} = \text{diag} (1, 1, -1)$. Since $\hat{U}$ is unitary, this mathematical transformation has no physical consequences.

The mapping between the Kane model and the $\alpha$-$T_3$ model shows that Kane fermions are hybrid pseudospin-1/2 and pseudospin-1 Dirac-Weyl fermions. The distinct chirality found in the 2D sectors A and B, respectively is mixed by the third dimension of dispersion, $k_z$. In this way, $k_z$ plays an analogous role to the mass $m$ in Eq. (3.9) which connects two chiral sectors in the 3D Dirac Hamiltonian. The difference is that in the 3D Dirac equation, the two chiral sectors are themselves 3D and connected by a constant mass factor rather than 2D sectors connected by a third component of dispersive momentum like in the Kane model.

**Kane Fermions in a Magnetic Field**

Under a magnetic field placed in the $z$-direction, the complex momentum $k_\pm (k_-)$ is replaced via the Peierls substitution with operators $\sqrt{2}a^\dagger/\ell_B \, (\sqrt{2}a/\ell_B)$. Then,

\[
\hat{H}_A = \gamma \begin{pmatrix}
0 & \sqrt{3}a & 0 \\
\sqrt{3}a^\dagger & E_g & -a \\
0 & -a^\dagger & 0
\end{pmatrix}, \quad \hat{H}_B = \gamma \begin{pmatrix}
0 & a & 0 \\
a^\dagger & E_g & -\sqrt{3}a \\
0 & -\sqrt{3}a^\dagger & 0
\end{pmatrix},
\]  

(3.80)
where \( \gamma = \hbar v / \sqrt{2} \ell_B \), and \( \bar{x} = x / \gamma \) wherever this notation occurs.

When restricted to 2D, sectors A and B are independent. The energy eigensystem for sector A, giving LL energies and their associated wavefunctions, is

\[
\tilde{\varepsilon}^A_{0,n} = 0, \quad n \geq 1 (n \neq 2); \\
\psi^A_{0,n} = \kappa \left( \sqrt{n-1}|n-3\rangle, 0, \sqrt{3(n-2)}|n-1\rangle \right)^T; \\
\tilde{\varepsilon}^A_{\xi,n} = (\bar{E}_g / 2) + \xi \sqrt{(\bar{E}_g / 2)^2 + 4n - 7}, \quad n \geq 2; \\
\psi^A_{\xi,n} = \kappa \left( \sqrt{3(n-2)}|n-3\rangle, \tilde{\varepsilon}^A_{\xi,n}|n-2\rangle, -\sqrt{n-1}|n-1\rangle \right)^T.
\]

The same for sector B is

\[
\tilde{\varepsilon}^B_{0,n} = 0, \quad n \geq 0 (n \neq 1); \\
\psi^B_{0,n} = \kappa \left( \sqrt{3n}|n-2\rangle, 0, \sqrt{n-1}|n\rangle \right)^T; \\
\tilde{\varepsilon}^B_{\xi,n} = (\bar{E}_g / 2) + \xi \sqrt{(\bar{E}_g / 2)^2 + 4n - 1}, \quad n \geq 1; \\
\psi^B_{\xi,n} = \kappa \left( \sqrt{n-1}|n-2\rangle, \tilde{\varepsilon}^B_{\xi,n}|n-1\rangle, -\sqrt{3n}|n\rangle \right)^T.
\]

The 2D LL energy distribution with \( E_g = 0 \) is plotted in Fig. 3.9 with red levels belonging to sector A and blue to sector B. Dashed lines in the figure trace out branches off of which the LL’s bud. It should be noted that the zero-energy LL’s at \( n = 3, 4, 5 \) are offset in the figure only for illustration.

As in the 2D Dirac-Weyl system, LL’s are proportional to \( \gamma \), giving them a \( \sqrt{B} \) dependence on the magnetic field. Another similarity is that for low \( n \), the available Hilbert space is restricted so that some LL’s are absent (such as the \( n = 2 \) level on the flat branch in sector A). In sector A, the Fock number index begins at \( n = 1 \) rather than \( n = 0 \). The reason for this is that the three-element wavefunctions in this 2D case are decomposed from the six-element 3D wavefunctions, retaining the numbering convention.

Allowing \( k_z \) to take finite values (and setting \( \hbar = v = 1 \) for brevity), the LL energies are no longer single points in Hilbert space but instead disperse along \( k_z \). The 3D Kane model...
Figure 3.9: Landau level (LL) energies for the 2D Kane model with $E_g = 0$. Red levels belong to sector A and blue to sector B. Dashed lines trace out the branches off of which the Landau levels bud. Some LL’s on the flat branch are vertically offset only for illustration.

LL energies are

$$\varepsilon^A_{0,n}(\bar{k}_z) = 0, \quad n \geq 1 (n \neq 2);$$
$$\varepsilon^A_{\xi,n}(\bar{k}_z) = (\bar{E}_g/2) + \xi \sqrt{(\bar{E}_g/2)^2 + \bar{k}_z^2 + 4n - 7}, \quad n \geq 2;$$
$$\varepsilon^B_{0,n}(\bar{k}_z) = 0, \quad n \geq 0 (n \neq 1);$$
$$\varepsilon^B_{\xi,n}(\bar{k}_z) = (\bar{E}_g/2) + \xi \sqrt{(\bar{E}_g/2)^2 + \bar{k}_z^2 + 4n - 1}, \quad n \geq 1. \quad (3.83)$$
The associated wavefunctions are

\[ \psi_{0,1}^A = \kappa \left( 0, 0, -\sqrt{3}|0\rangle, 0, 0, \bar{k}_z|1\rangle \right)^T, \]

\[ \psi_{0,n \geq 3}^A = \kappa \left( (\bar{k}_z^2 + n - 1)|n - 3\rangle, 0, \sqrt{3(n - 1)(n - 2)|n - 1\rangle, \sqrt{3(n - 2)}k_z|n - 2\rangle, 0, 0 \right)^T, \]

\[ \psi_{\xi,n}^A = \kappa \left( \sqrt{3(n - 2)|n - 3\rangle, \tilde{\epsilon}_{\xi,n}^A|n - 2\rangle, -\sqrt{n - 1}|n - 1\rangle, -\bar{k}_z|n - 2\rangle, 0, 0 \right)^T, \]

\[ \psi_{0,n}^B = \kappa \left( 0, 0, -\sqrt{3n}k_z|n - 1\rangle, \sqrt{3n(n - 1)|n - 2\rangle, 0, (k_z^2 + n - 1)|n\rangle \right)^T, \]

\[ \psi_{\xi,n}^B = \kappa \left( 0, 0, -\bar{k}_z|n - 1\rangle, \sqrt{n - 1}|n - 2\rangle, \tilde{\epsilon}_{\xi,n}^B|n - 1\rangle, -\sqrt{3n}|n\rangle \right)^T. \]

(3.84)

By setting \( k_z = 0 \) in this 3D eigensystem, the 2D eigensystem in Eqs. (3.81) and (3.82) is recovered. While 3D LL’s are given the labels A or B, these labels refer to distinct chiral sectors at \( k_z = 0 \) only.

The LL energies in Eq. (3.83) for \( E_g = 0 \) are plotted in Fig. 3.10 showing \( n \) and \( k_z \) dependence together up to \( n = 5 \). The back right panel provides a projection along the \( n \)-axis, showing only the \( k_z \) dependence of each level. The opposite panel shows the extremum of each band in \( k_z \), all of which are located at \( k_z = 0 \). This back-left panel is the same diagram as in Fig. 3.9. LL’s in sector A are coloured red, B in blue, and overlapping zero-energy levels are coloured purple.
Figure 3.10: Landau level (LL) energies for the 3D Kane model with $\vec{E}_g = 0$ showing $n$ and $k_z$ dependence up to $n = 5$. The back-right panel shows a projection along the $n$-axis, the back-left panel shows the $k_z$-extremum of each level. Sector A levels are in red, B in blue, and overlapping zero-energy levels are coloured purple.
Chapter 4

Dirac-Weyl Magneto-Optics

The magneto-optical conductivity of a general pseudospin-$s$ 2D Dirac-Weyl (DW) material is analyzed in this chapter. The specific cases of $s = \{1/2, 1, 3/2, 2\}$ are investigated and compared. Predictable patterns arise in the optical spectra which act as identifiable signatures of each system. The understanding of these patterns and of the general structure of various spectra is greatly aided by the invention of snowshoe diagrams. The findings reported in this chapter have been published in Ref. [57], from which many figures have been taken and are presented again here.

4.1 General Pseudospin-$s$

This chapter is concerned with the 2D Dirac-Weyl system in a magnetic field, detailed in Section 3.2. The state space is made up of non-dispersive LL’s, $\psi_{\lambda,n}$, labelled with a branch index, $\lambda$, and a Fock number, $n$. The LL wavefunctions for pseudospin up to $s = 2$ and corresponding energy eigenvalues are listed in Tables 3.3 and 3.2, respectively.

The general expression for the quantum many-body optical conductivity tensor under the RPA approximation is given in Eq. (2.33). For a 2D system in a magnetic field this expression becomes

$$
\sigma_{\alpha\beta}(\omega) = \frac{i\hbar}{2\pi e^2} \sum_{\lambda,\lambda', n,n'} \frac{n_f(\varepsilon_{\lambda,n}) - n_f(\varepsilon_{\lambda',n'}) \langle \psi_{\lambda,n} | \hat{j}_\alpha | \psi_{\lambda',n'} \rangle \langle \psi_{\lambda',n'} | \hat{j}_\beta | \psi_{\lambda,n} \rangle}{\hbar \omega - (\varepsilon_{\lambda',n'} - \varepsilon_{\lambda,n}) + i\eta},
$$

(4.1)
where
\[
j \equiv e \frac{\partial \hat{H}}{\partial (\hbar \mathbf{k})} = ev \hat{S}. \tag{4.2}\]

Note that the chemical potential, \(\mu\), is assumed to lie sufficiently far away from the energy of a LL. In this way, partial filling of LL’s and thus intra-level transitions are not considered. This, however, could be an interesting future consideration. The fractional quantum Hall effect (a feature in the reactive part of the optical conductivity) arises via interactions within partially filled LL’s, leading to fractionally charged excitations [47, 48]. Partial filling of the flat branch might be particularly interesting, where the already large degeneracy found in a single LL is greatly enhanced by having many of these LL’s all held at the same energy.

Of concern here are the absorptive parts of the conductivity tensor, \(\text{Re} \sigma_{xx}\) and \(\text{Im} \sigma_{xy}\). The inner products in Eq. (4.1) can be expanded using the general LL wavefunction in Eq. (3.20) and the spin-\(s\) matrices in Eq. (3.7), yielding
\[
\begin{align*}
\text{Re} \sigma_{xx}(\omega) &= \frac{ghe^2v^2}{8\ell_B^2} \sum_{\lambda,\lambda',n,n'} \frac{1}{\hbar \omega} \left[ n_f(\epsilon_{\lambda,n}) - n_f(\epsilon_{\lambda',n'}) \right] \delta(\hbar \omega - (\epsilon_{\lambda',n'} - \epsilon_{\lambda,n})) \\
\text{Im} \sigma_{xy}(\omega) &= \left( |f(\psi_{\lambda,n}; \psi_{\lambda',n'})|^2 \delta_{n',n-1} \pm |f(\psi_{\lambda',n'}; \psi_{\lambda,n})|^2 \delta_{n',n+1} \right),
\end{align*}
\tag{4.3}\]

where, with \(\rho_m = \sqrt{m(2s + 1 - m)}\),
\[
|f(\psi, \psi')|^2 = \left| \sum_{m=1}^{2s} \rho_m \alpha_m \alpha'_{m+1} \right|^2. \tag{4.4}\]

Explicit expressions for the overlap function, \(|f(\psi, \psi')|\), are given for the \(s = 1/2\) and \(s = 1\) systems in Table 4.1. Based on Eq. (4.3), a photon promotes the excitation of a filled LL, \(\psi_{\lambda,n}\), to an empty LL, \(\psi_{\lambda',n'}\) at a higher energy, with photon energy equal to the levels’ separation.

The behaviour in Eq. (4.3) can be made dimensionless by pulling out a factor of inverse squared energy, \(1/\gamma^2\), where the magnetic energy scale \(\gamma = hv/\sqrt{2}\ell_B \) goes as \(\sqrt{B}\). Also, for
Table 4.1: Explicit expressions for the overlap function, $|f(\psi, \psi')|^2$, for the $s = 1/2$ and $s = 1$ systems.

| $s$ | $(\psi, \psi')$ | $|f(\psi, \psi')|^2$ |
|-----|------------------|------------------|
| $1/2$ | $(\psi_{\pm,1}^1; \psi_0^0)$ | $1/2$ |
| | $(\psi_{\pm,\lambda,n+1}^1; \psi_{\lambda,n}^0 \geq 1)$ | $1/4$ |
| $1$ | $(\psi_{\pm,1}^1; \psi_0^0)$ | $1$ |
| | $(\psi_{\pm,1}^1; \psi_{0,n}^0 \geq 2)$ | $n-1/2n-1$ |
| | $(\psi_{0,n+1}^1; \psi_{\pm,1}^1)$ | $n+1/2n+1$ |
| | $(\psi_{\pm,\lambda,n+1}^1; \psi_{\lambda,\lambda,n}^0 \neq 0,n)$ | $(2n+\sqrt{4n^2-1})/4n^2$ |

Brevity, $\omega$ is taken to be the photon energy rather than the frequency (effectively dropping the $h$ factor). This leads to the somewhat cleaner expression

$$\begin{align*}
\text{Re} \sigma_{xx}(\omega) = & \frac{ge^2}{4\hbar} \sum_{\lambda,\lambda',n,n'} \frac{1}{\Omega} \left[ \tilde{n}_f(\tilde{\epsilon}_{\lambda,n}) - \tilde{n}_f(\tilde{\epsilon}_{\lambda',n'}) \right] \delta(\tilde{\omega} - (\tilde{\epsilon}_{\lambda',n'} - \tilde{\epsilon}_{\lambda,n})) \\
\text{Im} \sigma_{xy}(\omega) = & \frac{ge^2}{4\hbar} \sum_{\lambda,\lambda',n,n'} \frac{1}{\Omega} \left[ \tilde{n}_f(\tilde{\epsilon}_{\lambda,n}) - \tilde{n}_f(\tilde{\epsilon}_{\lambda',n'}) \right] \delta(\tilde{\omega} - (\tilde{\epsilon}_{\lambda',n'} - \tilde{\epsilon}_{\lambda,n})) \\
\times & \left( |f(\psi_{\lambda,n}; \psi_{\lambda',n'})|^2 \delta_{n',n-1} \pm |f(\psi_{\lambda',n'}; \psi_{\lambda,n})|^2 \delta_{n',n+1} \right),
\end{align*}$$

(4.5)

where a dimensionless parameter uses the notation $\bar{x} = x/\gamma$ along with the function $\tilde{n}_f(\bar{x}) = n_f(x)$. The dimensionful factor out front involves the quantum of conductivity in 2D, $e^2/h$, and the degeneracy factor $g$. For the DW systems emergent in both graphene and the dice lattice, $g = 4$ because of the two-fold intrinsic spin degeneracy and two-fold valley degeneracy.

Note that in the overlap function $|f(\psi, \psi')|^2$, the first argument, $\psi$, will always have the larger Fock number. LL wavefunctions $\psi_{\lambda,n}$ and $\psi_{-\lambda,n}$ are the same except for a negative factor on the even elements of the latter spinor. This leads to the mirrorymmetric property of the overlap function,

$$|f(\psi_{\lambda,n+1}; \psi_{\lambda',n'})|^2 = |f(\psi_{-\lambda,n+1}; \psi_{-\lambda',n'})|^2,$$

(4.6)

which is a manifestation of the particle-hole symmetry in the DW system.
The evaluation of the current operators in the DW system (leading to Eq. (4.5)) demonstrates the strict selection rule $n' = n \pm 1$. This is different from the zero-field ($B = 0$) rule, $\lambda' = \lambda \pm 1$. For finite $B$, $\lambda$ is no longer a good quantum and cannot be involved in a strict selection rule. However, as is demonstrated below for specific cases, $\Delta \lambda > 1$ transitions have a minor contribution to the magneto-optics, making $\lambda' = \lambda \pm 1$ a weak selection rule.

For right- and left-handed circular polarized light the absorptive part of the conductivity is, respectively,

$$\text{Re } \sigma_{\pm}(\omega) = \text{Re } \sigma_{xx}(\omega) \mp \text{Im } \sigma_{xy}. \quad (4.7)$$

As such, right-handed light can only promote transitions to higher Fock number ($n \to n + 1$) while left-handed light does the opposite ($n \to n - 1$).

### 4.2 $s = 1/2$

The magneto-optics of the $s = 1/2$ system have been discussed extensively in the context of graphene [51,58,59], where these effects have also been measured and confirmed [60–63]. This system is studied so prolifically that many extensions of Eq. (4.5) have been made which include the effects of electron-phonon coupling [64], the effects of a potential difference between sublattices and an appreciable spin-orbit coupling (applicable to silicene, a buckled honeycomb lattice of silicon atoms) [65,66], and the effects of a quadratic-in-momentum term in the Hamiltonian (applicable to topological insulator surface states) [67]. Despite previous analyses, the magneto-optical conductivity for $s = 1/2$ based on Eq. (4.5) is again detailed here, allowing for a direct comparison with the higher-pseudospin systems discussed later. It also provides the simplest platform to introduce snowshoe diagrams and other ideas pertaining to the analysis of each spectrum.

A snowshoe diagram takes the LL energy spectrum, as in Fig. 3.2, and ‘laces it up’ by sketching in all of the allowed transitions between levels based on a particular $\mu$. These transitions obey the selection rule $n \to n \pm 1$ and the Pauli exclusion principle. In Fig. 4.1, snowshoe diagrams are given for the $s = 1/2$ system under three different chemical potential, $\mu$, illustrated with a black horizontal line in each panel. Going from left to right, the panels show sequential filling of LL’s starting with the special zero-energy level, $\psi_{0,0}$. The arrows
Figure 4.1: Snowshoe diagrams for the $s = 1/2$ DW system under three different chemical potentials, marked with a horizontal black line. Blue arrows show allowed intra-branch transitions between LL’s and red show inter-branch transitions. Note that the blue transition in panel (a) can also be considered as inter-branch due to the ambiguous nature of the $n = 0$ Landau level.

Drawn in each diagram represent a transition from a filled LL to an empty one. The vertical length of the arrow measures the energy of the transition, which can only move one step to the left or right ($n \to n \pm 1$). Inter-branch transitions are coloured red and intra-branch in blue.

Without loss of generality, $\mu$ in this chapter is always taken to be positive. Due to particle-hole symmetry of the DW system, the conductivity is invariant to a sign change in $\mu$. In this transformation ($\mu \to -\mu$), the snowshoe diagrams are reflected about $\varepsilon = 0$ and $\Re \sigma_{xx}$ is left the same. The sign on $\Im \sigma_{xy}$ is flipped and the circular polarization spectra $\Re \sigma_+$ and $\Im \sigma_-$ are swapped. This is the same for all DW systems, not just $s = 1/2$, and is summarized in Table 4.2.

Note that the energy of LL’s is proportional to $\sqrt{B}$. Then, the filling of LL’s by increasing $\mu$ at a fixed $B$ can also be achieved by decreasing $B$ at a fixed $\mu$. This latter approach, however, would change the energy scale on which the optical conductivity depends. Peaks associated with distinct transitions would be pushed closer together, making them more difficult to resolve in an experiment.

In Fig. 4.1(a), none of the inter-branch transitions ($\lambda = -1/2 \to +1/2$, red) are blocked.
Table 4.2: Effect on different components in the magneto-optical conductivity upon the transformation $\mu \to -\mu$. This applies to any system with particle-hole symmetry.

<table>
<thead>
<tr>
<th>$\mu$</th>
<th>$-\mu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Re \sigma_{xx}$</td>
<td>$\Re \sigma_{xx}$</td>
</tr>
<tr>
<td>$\Im \sigma_{xy}$</td>
<td>$-\Im \sigma_{xy}$</td>
</tr>
<tr>
<td>$\Re \sigma_{+}$</td>
<td>$\Re \sigma_{-}$</td>
</tr>
<tr>
<td>$\Re \sigma_{-}$</td>
<td>$\Re \sigma_{+}$</td>
</tr>
</tbody>
</table>

These transitions come in pairs, equal in energy and mirror-symmetric about $\varepsilon = 0$. The partner to the general transition ($\psi_{-\frac{1}{2},n} \to \psi_{\frac{1}{2},n+1}$) is ($\psi_{-\frac{1}{2},n+1} \to \psi_{\frac{1}{2},n}$). By filling an additional LL in the next panel of the figure, one of the transitions in the first pairing is locked out, while all other inter-branch pairs remain unchanged. At the next filling in panel (c), the remaining transition in the first pair is locked out, in addition to one of the transitions in the next pairing. This trend continues as LL’s are successively filled, always leaving a single unpaired inter-branch transition and a series of paired transitions.

In each panel of Fig. 4.1, there is only one allowed intra-branch transition. Moving from left to right, the energy difference between the states involved decreases as LL’s are filled. The first of these transitions, shown panel (a), is distinct because it arises from the special state $\psi_{0,0}$ which is shared between branches. As such, it could be labelled as both an intra- and inter-branch transition [51]. However, for discussions around the patterns in the conductivity as LL’s are filled, this transition groups well with the intra-branch transitions.

Particle-hole symmetry dictates that any mirror-symmetric pair of arrows must have equal contribution, shown in the identity Eq. (4.6). Then, from Eq. (4.5), a mirror-symmetric pair will interfere constructively in $\Re \sigma_{xx}$ and destructively in $\Im \sigma_{xy}$. These functions are plotted in Figs. 4.2 and 4.3, respectively, which use $\Omega = \omega$ as the photon energy. Each panel in these figures is the conductivity associated with the corresponding snowshoe diagram in Fig. 4.1. For a more realistic curve, and one that is legible, the delta

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function in Eq. (4.5) has been replaced with a Lorentzian,

$$\delta(x) \rightarrow L(x) = \frac{\eta/\pi}{x^2 + \eta^2}$$

which is a peak that envelops a total area of 1 and has a width $\eta$. Taking $\eta \rightarrow 0$ retrieves the delta function. In the figures, a width $\eta = 0.03$ has been chosen for aesthetic reasons. All of the spectra in this chapter plot the conductivity at zero temperature where the Fermi-Dirac distribution is simply a step function,

$$n_f(x)\bigg|_{k_BT=0} = \Theta(\mu - x).$$

(4.9)

The temperature $k_BT$ gives the scale about $\mu$ on which $n_f(x)$ shows curvature. Then Eq. (4.9) can still be a good approximation at finite temperatures, provided that the separation between $\mu$ and the energy of any LL is much larger than $k_BT$,

$$|\mu - \varepsilon_{\lambda,n}| \gg k_BT \text{ for all } \lambda, n.$$  

(4.10)

Each spectrum in Figs. 4.2(a)-(c) show a single intra-branch peak (blue) appearing with greater amplitude and at a lower energy in each successive panel. Seen in the snowshoe diagrams, there is a single intra-branch transition in each panel, with the energy separation getting smaller as LL’s get filled. The change in amplitude in these blue peaks comes from the $1/\bar{\omega}$ factor on each transition in Eq. (4.5), increasing the amplitude for lower photon energy.

In Fig. 4.2(a), there is a series of inter-branch peaks (red) whose amplitudes follow a monotonic decline with increasing energy. Each peak corresponds to a pair of mirror-symmetric transitions in Fig. 4.1(a), where each transition in a pair contributes an equal weighting to the peak. In the next panel, following down the first dashed line, the first red peak is exactly halved in height, while the others in the series remain unchanged. This corresponds to the locking out of a single transition in the first pair in the corresponding snowshoe diagram. In the final panel, both transitions in the first pair are locked out, removing this peak altogether. In addition, a single transition in the next pair is locked.
Figure 4.2: Absorptive part of the longitudinal conductivity in the $s = 1/2$ DW system. Each panel gives the conductivity associated with the corresponding snowshoe diagram in Fig. 4.1. Blue peaks correspond to intra-branch transitions and red to inter-branch transitions. Vertical dashed lines trace the locations of peaks discussed in the text.
Figure 4.3: Absorptive part of the transverse conductivity in the $s = 1/2$ DW system. Labels are as in Fig. 4.2.
out, so that the next peak is halved in height (second dashed line in the spectrum). This pattern repeats: as a LL is filled, the half-height peak will disappear and the peak to its right will be halved in height.

In the off-diagonal component, Fig. 4.3, right-directed transitions \( n \to n+1 \) come with an overall negative sign on the peak according to Eq. (4.5). The left-directed transitions \( n \to n - 1 \), on the other hand, all make a positive contribution to the spectrum. As such, mirror-symmetric pairs of arrows in a snowshoe diagram, with equal weighting, will exactly cancel out in this spectrum. In the first panel, where there are no unpaired inter-branch transitions, the single peak in the spectrum is only due to the intra-branch transition. As LL’s are successively filled, the unpaired inter-branch transition gives a single red peak in each of the panels (b) and (c).

Figures 4.4 and 4.5 plot the absorptive part of the optical conductivity for the right- and left-handed circular polarization using Eq. (4.7). For positive chemical potential, all intra-branch transitions are right directed \( n \to n + 1 \), appearing only in the spectrum for right-handed polarization. Also, each transition in a mirror-symmetric pair contributes to separate spectra. As each positive-energy LL is successively filled, the left-directed transition is the first in a pair to be locked out. Then the peak at this energy first disappears in \( \text{Re} \sigma_- \) (without any halving). In the other spectrum, \( \text{Re} \sigma_+ \), the peak disappears at the next filling of a LL.

The patterns seen in the \( s = 1/2 \) magneto-optics are well established and simple to understand. As more branches are added to the system with higher values of pseudospin, variety in the different types of transitions that occur leads to more complex spectra. However, with the aid of snowshoe diagrams, patterns can be identified. In turn, these patterns act as identifiers for each unique system.

### 4.3 \( s = 1 \)

Snowshoe diagrams showing successive filling of positive LL’s in the \( s = 1 \) system are presented in Figs. 4.6(a)-(c). The green transitions \( (\lambda = -1 \to +1) \) come in mirror-symmetric pairs like the red transitions in Fig. 4.1, leading to the same spectral patterns as
Figure 4.4: Absorptive part of the optical conductivity for right-handed circular polarization in the $s = 1/2$ DW system. Labels are as in Fig. 4.2.
Figure 4.5: Absorptive part of the optical conductivity for left-handed circular polarization in the $s = 1/2$ DW system. Labels are as in Fig. 4.2.
the $s = 1/2$ inter-branch transitions. However, these transitions in the $s = 1$ system occur at a larger energy (notice that the vertical scale in Fig. 4.6 is about twice that in Fig. 4.1). Also, the transition has a branch separation $\Delta \lambda > 1$, leading to a suppression of the peak. This is residual of the strict selection rule at zero field $\Delta \lambda = \pm 1$.

Transitions out of the flat-branch come in equal-energy pairs, but these pairs are not mirror symmetric about $\varepsilon = 0$. Instead, each pair forms an isosceles triangle where both transitions terminate on the same state. It is important to point out that the state $\psi_{1,2}$ (the second positive LL) is the terminus of only one such transition due to the absence of an $n = 1$ state in the flat branch. Thus, out of the full series of available flat-branch transitions, the only one unpaired in panel (a) of the figure is $(\psi_{0,3} \rightarrow \psi_{1,2})$.

$\Re \sigma_{xx}$ and $\Im \sigma_{xy}$ for the $s = 1$ system are plotted in Figs. 4.7 and 4.8, showing marked differences from their counterparts in the well-known $s = 1/2$ system, Figs. 4.2 and 4.3, respectively. The colouring of the peaks in these spectra match the colouring in the $s = 1$ snowshoe diagrams, Fig. 4.6.

At the first chemical potential considered, the $\lambda = +1$ branch is completely empty so that there are no intra-branch peaks in Figs. 4.7(a) and 4.8(a). Once the first positive LL is
Figure 4.7: Absorptive part of the longitudinal conductivity in the $s = 1$ DW system. Each panel gives the conductivity associated with the corresponding snowshoe diagram in Fig. 4.6. Blue peaks correspond to intra-branch transitions, red to $\Delta \lambda = 1$ inter-branch transitions, and green to $\Delta \lambda = 2$. Vertical dashed lines trace the locations of peaks discussed in the text.
Figure 4.8: Absorptive part of the transverse conductivity in the $s = 1$ DW system. Labels are as in Fig. 4.7.
filled, a single intra-branch peak appears in each spectrum, appearing at lower energy and
with larger amplitude as LL’s are successively filled. This is the same intra-branch peak
pattern seen in the $s = 1/2$ system.

The $\lambda = -1 \rightarrow +1$ peaks (green) in Fig. 4.7 show the same patterns of the mirror-
symmetric transitions in $s = 1/2$ ($\lambda = -1/2 \rightarrow +1/2$). On the energy scale shown in the
$s = 1$ plots, only one such peak appears, located at an energy slightly less than $\omega = 4\gamma$. In
going from panel to panel, this peak (along the third dashed line) is first halved in height
and then disappears completely. For the transverse conductivity, this peak only appears in
Fig. 4.8(b) when there is a single unpaired transition in the snowshoe diagram.

Transitions from the flat branch (red) make up the majority of features in the $s = 1$
spectra. In general, both transitions that contribute to a single red peak have the same
terminal state. The locations of the peaks land on the exact energies of the upper branch.
As a level is filled, the peak in Re $\sigma_{xx}$ associated with the transition completely disappears
without any halving, such as the first red peak seen along the first dashed line in Fig. 4.7.
The second peak in panel (a) is rather interesting, as it does not fit in with the rest of the
peaks in the series. This is the single flat-branch transition in which only one transition
contributes instead of two, breaking the otherwise monotonic decline of the peaks. This
non-monotonic decline of peaks in Re $\sigma_{xx}$ is a clear and identifying structure in the
$s = 1$ spectrum.

The equal-energy pairs of flat-branch transitions are not mirror symmetric. As such,
their associated overlap functions are not equal and do not cancel in Im $\sigma_{xy}$. Instead, the
dominant transition in each pair wins out. In general, it is the left-directed transition,
($\psi_{0,n+1} \rightarrow \psi_{1,n}$), that dominates over the right-directed transition, ($\psi_{0,n-1} \rightarrow \psi_{1,n}$), giving
a series of positive peaks in Fig. 4.8. To demonstrate this, Table 4.1 is used to calculate the
difference in the overlap function contributions,

$$
|f(\psi_{0,n+1};\psi_{1,n})|^2 - |f(\psi_{1,n};\psi_{0,n-1})|^2 = \frac{n+1}{2n+1} - \frac{n-2}{2n-3} = \frac{2n-1}{(2n-3)(2n+1)} \quad (n \geq 3),
$$

which is greater than zero (for general $n \geq 3$). However, the lowest-energy pair involves the
right-directed transition out of the special state $\psi_{0,0}$ which dominates over the left-directed transition,
\[ |f(\psi_{0,2}; \psi_{1,1})|^2 - |f(\psi_{1,1}; \psi_{0,0})|^2 = \frac{2}{3} - 1 = -\frac{1}{3}, \]
(4.12)
giving the single negative peak in Fig. 4.8(a). The second peak in this figure is positive and quite large. This is because the peak comes from that single left-directed transition which has no right-directed pair to reduce the height of its peak.

Circular polarizations $\text{Re} \sigma_+$ and $\text{Re} \sigma_-$ in Figs. 4.9 and 4.10, respectively, show the difference and sum of $\text{Re} \sigma_{xx}$ and $\text{Im} \sigma_{xy}$. $\text{Re} \sigma_+$ reveals peaks for all right-directed transitions and $\text{Re} \sigma_-$ for all the left-directed ones. As such, $\text{Re} \sigma_-$ shows no intra-branch peaks (for
Figure 4.10: Absorptive part of the optical conductivity for left-handed circular polarization in the $s = 1$ DW system. Labels are as in Fig. 4.7.
\( \mu > 0 \). The flat-branch transitions give the same series of peaks in either polarization except for the second peak (along the second dashed line) which is absent from \( \text{Re}\,\sigma_+ \), owing to the lack of a right-directed transition into the state \( \psi_{1,2} \). This absent peak in one of the circular polarizations is yet another signature of \( s = 1 \). The amplitudes of the peaks in these series are different in either polarization due to the unequal weighting in the overlap functions with right- and left-directed transitions. The appearance and disappearance of peaks as LL’s are filled are easily understood from the snowshoe diagrams, as in the \( s = 1/2 \) system.

4.4 \( s = 3/2 \)

With two positive and two negative LL branches, the \( s = 3/2 \) system becomes increasingly complicated. Also, there are now two special zero-energy levels, \( \psi_{0,0} \) and \( \psi_{0,2} \). The snowshoe diagrams for this system at four different fillings are given in the panels of Fig. 4.11. In the first panel, the positive-energy levels are all empty. As \( \mu \) increases between subsequent panels, the \( \lambda = +1/2 \) branch has its first two levels filled in succession in panels (b) and (c) followed by the first level in the \( s = +3/2 \) branch in panel (d). In these last three panels, it is difficult to discern a large change in the black line marking \( \mu \). A better indication is the fact that all transitions come out of the filled LL sea and terminate in an empty state.

Figure 4.12 gives the longitudinal conductivities, \( \text{Re}\,\sigma_{xx} \), associated with each snowshoe diagram in Fig. 4.11. The two sets of intra-branch transitions \( (\lambda = -1/2 \rightarrow +1/2) \) and \( (\lambda = -3/2 \rightarrow +3/2) \) come in the same mirror-symmetric pairs as the \( s = 1/2 \) inter-branch transitions (Fig. 4.1). Then the spectral peaks associated with these transitions all show the same patterns upon LL filling. Starting from low energy, a peak is first halved and then disappears totally. As the peak to its left disappears, a full peak goes to half height. This is seen along the vertical dashed lines in Fig. 4.12 for peaks coming from transitions between the \( |\lambda| = 1/2 \) branches. The change in the spectrum between panels (c) and (d) is due to the filling of a level in the \( \lambda = +3/2 \). This has no effect on the peak along the second dashed line, explaining why it has not yet disappeared.

Transitions in the full set \{\( (\lambda = -1/2 \rightarrow +3/2), (\lambda = -3/2 \rightarrow +1/2) \)\} also come
Figure 4.11: Snowshoe diagrams for the $s = \frac{3}{2}$ DW system under four different chemical potentials, marked with a horizontal black line. Blue arrows show $\Delta \lambda = 0$ transitions, red show $\Delta \lambda = 1$, green show $\Delta \lambda = 2$, and cyan show $\Delta \lambda = 3$. 
Figure 4.12: Absorptive part of the longitudinal conductivity in the $s = 3/2$ DW system. Each panel gives the conductivity associated with the corresponding snowshoe diagram in Fig. 4.6, sharing the same colouring convention between figures. Vertical dashed lines and arrows mark the locations of peaks discussed in the text.
in mirror-symmetric pairs. As such, the associated peaks obey this same halving-and-disappearance pattern seen for any series of peaks composed of mirror-symmetric transitions. However, along with the transitions between $|\lambda| = 3/2$ branches, the large separations in energy and branch index means these transitions have little effect on the conductivity (small green and cyan peaks in Fig. 4.12).

This system also allows for the possibility of transitions between the two positive-energy branches. This set of transitions produces peaks that wholly appear and then disappear without halving due to any lack of symmetry. Specifically, as a LL with $\lambda = +1/2$ becomes occupied, two transitions out of it can occur which terminate in different $\lambda = +3/2$ states. This causes two separated peaks to appear in the spectrum at once, such as the two red peaks indicated with arrows in Fig. 4.12(b) and another pair indicated with the two arrows on the right in panel (c). In each pair, the lower energy peak disappears first as its terminal LL becomes filled. This is seen between panels (c) and (d) in the disappearance of the peak indicated with the leftmost arrow in the first panel.

Based on the analysis in previous sections, the transverse conductivity $\text{Im} \sigma_{xy}$ will display peaks for all transitions that are not cancelled out by a mirror-symmetric pair. Transitions directed to the left will manifest as positive peaks and right-directed transitions to negative peaks. For the two degenerate peaks at an energy $\omega \sim 1.7$, the red peak comes from a left-directed transition and blue from a right-directed one. Because the blue peak is larger, its negative contribution will dominate the positive contribution over the red peak in the transverse conductivity. Spectra for circular polarizations, $\text{Re} \sigma_+$ and $\text{Re} \sigma_-$ will display peaks associated with right- and left-directed transitions respectively.

By now the analysis of these additional spectra ($\text{Im} \sigma_{xy}$, $\text{Re} \sigma_+$, and $\text{Re} \sigma_-$) should be well established. Of more interest here is the effect that the different values of pseudospin have on the general magneto-optics, rather than the difference between specific spectra at a particular value of $s$. As such, from here on it suffices to go into depth for the analysis of $\text{Re} \sigma_{xx}$ only.
Figure 4.13: Snowshoe diagrams on the $s = 2$ DW system showing the four different types of transitions based on their symmetry. These types are (a) intra-branch, (b) mirror-symmetric pairs, (c) flat-branch, and (d) asymmetric. While all transitions in this figure come in mirror symmetric pairs, this is only retained in panel (b) once a chemical potential is specified. Blue arrows show $\Delta \lambda = 0$ transitions, red show $\Delta \lambda = 1$, green $\Delta \lambda = 2$, cyan $\Delta \lambda = 3$, and purple $\Delta \lambda = 4$.

4.5 $s = 2$

In the final system analyzed, the $s = 2$ LL spectrum has more than one positive energy branch (with their negative counterparts) plus a flat band. Accordingly, this system includes the four different types of transition discussed thus far. Each type contributes its own spectral pattern to the optical conductivity. Furthermore, these four sets encompass all transitions that can occur in any general-peudospin DW system, including those with $s > 2$.

The four types of transition are illustrated as snowshoe diagrams in the panels of Fig. 4.13. These diagrams do not consider Pauli blocking of transitions, but instead display each full set. By imposing a chemical potential, many of the transitions illustrated are
Figure 4.14: Absorptive part of the longitudinal conductivity in the $s = 2$ DW system for the filling of four successive positive LL’s. Colouring of peaks uses the same convention as in Fig. 4.13. Vertical dashed lines and arrows mark the locations of peaks discussed in the text.
locked out. Figure 4.14 gives the longitudinal conductivity, $\text{Re } \sigma_{xx}$ under the successive filling of three LL's: $\psi_{+1,3}$ (panel (a) to (b)), $\psi_{+2,1}$ ((b) to (c)), and $\psi_{+1,4}$ ((c) to (d)).

The first type of transition identified is the set of intra-branch transitions (Fig. 4.13(a)), which cannot occur in the flat branch. When specifying a chemical potential, only a maximum of two such transitions can occur in the $s = 2$ system. A single peak in $\text{Re } \sigma_{xx}$ associated with an intra-branch transition will be replaced by a larger peak at lower energy as the next LL on the branch is filled. Two such peaks are labelled with their branch index in Fig. 4.14(d).

The next type are the mirror-symmetric transitions, shown in Fig. 4.13(b). While all panels in the figure display mirror-symmetric pairs, once the chemical potential is considered this is only retained for transitions in panel (b). Each transition in a pair contributes an equal weight to a single peak in the $\text{Re } \sigma_{xx}$ spectrum. As one transition is locked out, this peak is halved. The peak then disappears as the terminal state in the next transition is filled. At the same time, this filling will halve a similar peak located at higher energy. For the limited energy in Fig. 4.14, only one such peak appears, indicated with the rightmost vertical dashed line. Between panels (a) and (b), this peak loses half its height. It then disappears between panels (c) and (d).

The third type, flat-branch transitions, includes all transitions involving the flat branch, Fig. 4.13(c). For the $s = 2$ system, there are two different series of equal-energy pairs of transitions: one with $\Delta \lambda = 1$ (red) and the other with $\Delta \lambda = 2$ (green). Each series corresponds to a string of peaks in $\text{Re } \sigma_{xx}$ which show a ‘flat-branch signature’ similar to the $s = 1$ system. For transitions $\lambda = 0 \rightarrow +1$, the pattern is exactly the same. The second peak in the series is seemingly reduced because it only has one contributory transition terminating in the $n = 4$ state. In the $\lambda = 0 \rightarrow +2$ set, we see that, as in the other branch, there is only one transition terminating in the $n = 4$, leading to a reduced-height peak at the energy $\omega = \varepsilon_{+2,4} \approx 6.5\gamma$ (beyond the energy scale in plot). In addition, the $n = 2$ level has no flat-branch states to its left or right. Then there is no ‘second’ peak in the spectrum. The counting here refers to the absence of a peak in the location of the second LL in the branch, $\omega = \varepsilon_{+2,2} \approx 3.7\gamma$; it does not refer to the second peak actually observed.

For any integer-$s$ system, there are different series of peaks associated with transitions
from the flat-branch into each positive-energy branch $\lambda$. There are no transitions into any state with even-valued $n < 2s$. The $n = 2s$ states in all positive-energy branches each have just one flat-branch transition, giving the reduced-height peak in the spectrum. Then, for a series based on the branch $\lambda$, there will be $\lambda - 1$ absent peaks at alternating locations. At the location $\omega = \varepsilon_{\lambda,2s}$, the peak in the series has a reduced height. Beyond this, all of the peaks in the series follow a monotonic decline in amplitude, with none that are absent.

The final type are the asymmetric transitions (Fig. 4.13(d)) with $\lambda \rightarrow \lambda'$, where $\text{sgn} \lambda = \text{sgn} \lambda'$. This category includes the $\lambda = +1/2 \rightarrow +3/2$ transitions seen in the $s = 3/2$ system. For positive chemical potential, as the initial state is filled, two separate peaks appear at once in the spectrum. Each of these peaks disappear at different instances as their terminal states become occupied. The arrows in Figs. 4.14(b) and in panel (d) indicate the appearance of such pairs of peaks.

These four types of transitions appearing in the $s = 2$ can be used to describe LL transitions in any DW system: intra-branch, mirror-symmetric, flat-branch, or asymmetric. Breaking a complicated spectrum down into its different contributions makes the analysis simpler, particularly with the aid of snowshoe diagrams. The analysis in this chapter has described various identifiable signatures present in the various DW optical spectra (such as the non-monotonic decline in flat-branch peak amplitudes). These signatures can be used to classify potential relativistic materials based on their pseudospin through experiment.
Chapter 5

Kane Fermion Magneto-Optics

Not all relativistic materials are described exactly by the Dirac equation. In a broader sense, a relativistic material is described by the linear-in-momentum energy dependence in its quasiparticle behaviour. The Kane fermions introduced in Chapter 3 fit this criteria for zero gap, $E_g = 0$. Dirac and Kane fermions share other similarities as well. When restricted to 2D, the Kane system is chiral, much like the 3D Dirac equation when the mass is constrained to zero. Massless Kane fermions ($E_g = 0$) also exhibit Klein tunnelling (zero back scattering off of an arbitrarily high potential barrier) [29].

In this chapter, analytic expressions are derived for the magneto-optical conductivity of Kane fermions. This is first done restricted to 2D only, then for the full 3D system. Hg$_{1-x}$Cd$_x$Te (MCT), being host to massless Kane fermions at a critical Cd:Te ratio, $x = x_c \approx 0.17$, is also studied. At the end of the chapter, the optical conductivity of MCT is calculated, successfully matching measurements from experiment.

The information reported in this chapter as well as many of the figures can be found in Refs. [24,68].

5.1 2D Magneto-Optics

The magneto-optical conductivity for the $\alpha$-$T_3$ model has been derived elsewhere [27,69], whose results apply to the 2D Kane system using the specific value $\alpha = 1/\sqrt{3}$. The calculation done in this section is for reference to the 3D Kane magneto-optics derived later.

The general expression for the optical conductivity tensor in the RPA approximation for a 2D system in a magnetic field is given in Eq. 4.1. As applied to the Kane system
(Eqs. (3.81) and (3.82)), the absorptive parts of the conductivity are

\[
\begin{aligned}
\text{Re} \sigma_{xx}(\omega) &= \frac{ge^2}{4\hbar} \sum_{\zeta=A,B} \sum_{\lambda,\lambda'} \frac{1}{\bar{\omega}} \left[ \bar{n}_f(\bar{\varepsilon}_{\lambda,n}) - \bar{n}_f(\bar{\varepsilon}_{\lambda',n'}) \right] \delta \left( \bar{\omega} - (\bar{\varepsilon}_{\lambda',n'} - \bar{\varepsilon}_{\lambda,n}) \right) \\
\text{Im} \sigma_{xy}(\omega) &= \frac{ge^2}{4\hbar} \sum_{\zeta=A,B} \sum_{\lambda,\lambda'} \frac{1}{\bar{\omega}} \left[ \bar{n}_f(\bar{\varepsilon}_{\lambda,n}) - \bar{n}_f(\bar{\varepsilon}_{\lambda',n'}) \right] \delta \left( \bar{\omega} - (\bar{\varepsilon}_{\lambda',n'} - \bar{\varepsilon}_{\lambda,n}) \right) \\
&\quad \times \left( |f^c(\psi_{\lambda,n};\psi_{\lambda',n'})|^2 \delta_{n',n-1} \pm |f^c(\psi_{\lambda',n};\psi_{\lambda,n})|^2 \delta_{n',n+1} \right). \\
\end{aligned}
\]

According to Eq. (5.1), the familiar LL selection rule is obeyed, \( n \rightarrow n \pm 1 \). Also, there are no inter-sector contributions to the conductivity (A\( \leftrightarrow \)B), with different overlap functions within each chiral sector,

\[
|f^A(\psi,\psi')|^2 = |\sqrt{3} \alpha_1 \alpha'_2 - \alpha_2 \alpha'_3|^2, \quad |f^B(\psi,\psi')|^2 = |\alpha_1 \alpha'_2 - \sqrt{3} \alpha_2 \alpha'_3|^2.
\]

Recall that in 2D, the two sectors are disjoint (\( \hat{H} = \hat{H}_A \oplus \hat{H}_B \)). The degeneracy factor, \( g = 2 \), only includes the intrinsic-spin degeneracy since sectors A and B do not make the same contribution to the conductivity.

In addition to considering separate contributions from the two sectors, it is useful to break the conductivity down further into flat-cone (FC) and cone-cone (CC) pieces (appropriating the term ‘cone’ from the zero-field band structure). FC refers to all transitions either into or out of the flat-branch, and CC to the intra- and inter-branch transitions involving finite-energy branches (cones) only,

\[
\begin{aligned}
\text{Re} \sigma_{xx}(\omega) &= \frac{ge^2}{4\hbar} \sum_{\zeta=A,B} \left[ (FC)^c_{xx} + (CC)^c_{xx} \right], \\
\text{Im} \sigma_{xy}(\omega) &= \frac{ge^2}{4\hbar} \sum_{\zeta=A,B} \left[ (FC)^c_{xy} + (CC)^c_{xy} \right].
\end{aligned}
\]

Because of the gap parameter, \( E_g \), there is no particle-hole symmetry in general (only for \( E_g = 0 \)). As such, a full range of chemical potential must be considered; it does not suffice to consider \( \mu > 0 \) only.
Figure 5.1: Snowshoe diagrams in the 2D Kane system separating out those in sectors A and B (panels (a) and (b), respectively). These diagrams correspond to the spectrum in Fig. 5.2. Sector A is coloured red, sector B in blue, and the uninvolved sector in each panel has been shaded grey. The chemical potential $\mu = \gamma/2$ is marked in green.
Sector A

In this subsection the label A is dropped since all of the work is done in that sector. Considering all of the different transitions involving the flat branch,

\[(FC)_{x,y} = \sum_{\xi = \pm} \left( (\delta_{\xi,+} \pm \delta_{\xi,-}) \sum_{n=2}^{\infty} \left| \frac{\tilde{n}_f(0) - \tilde{n}_f(\bar{\varepsilon}_{\xi,n})}{\bar{\varepsilon}_{\xi,n}} \right| |f(\psi_{0,n+1}; \psi_{\xi,n})|^2 \delta(\bar{\omega} - |\bar{\varepsilon}_{\xi,n}|) \right. \\
+ (\delta_{\xi,-} \pm \delta_{\xi,+}) \left| \frac{\tilde{n}_f(0) - \tilde{n}_f(\bar{\varepsilon}_{\xi,2})}{|\bar{\varepsilon}_{\xi,2}|} \right| |f(\psi_{\xi,2}; \psi_{0,1})|^2 \delta(\bar{\omega} - |\bar{\varepsilon}_{\xi,2}|) \\
+ \left( \frac{\varepsilon_{0,n}}{\bar{\varepsilon}_{\xi,n+1}} \right) \sum_{n=3}^{\infty} \left| \frac{\tilde{n}_f(0) - \tilde{n}_f(\bar{\varepsilon}_{\xi,n+1})}{|\bar{\varepsilon}_{\xi,n+1}|} \right| |f(\psi_{\xi,n+1}; \psi_{0,n})|^2 \delta(\bar{\omega} - |\bar{\varepsilon}_{\xi,n+1}|) \right) .
\]

(5.4)

The first line includes all of the transitions in which the flat-branch LL involved is on the right \( (\psi_{\pm,n} \leftrightarrow \psi_{0,n+1}) \). The other two lines have the zero-energy LL on the left \( (\psi_{0,n} \leftrightarrow \psi_{\pm,n+1}) \), skipping over the \( n = 2 \) term due to the absence of a zero-energy LL at that location. Snowshoe diagrams, like in Fig. 5.1, are a good aid in keeping track of which transitions terms are to be included.

The overlap functions in Eq. (5.4) are

\[|f(\psi_{0,n+1}; \psi_{\pm,n})|^2 = \frac{3n(\bar{\varepsilon}_{\pm,n})^2}{((\bar{\varepsilon}_{\pm,n})^2 + (4n-7))(4n-3)},\]

\[|f(\psi_{\pm,n+1}; \psi_{0,n})|^2 = \frac{3(n-2)(\bar{\varepsilon}_{\pm,n+1})^2}{(4n-7)((\bar{\varepsilon}_{\pm,n+1})^2 + (4n-3))}.\]

(5.5)

Note that the latter expression is zero for \( n = 2 \), which allows us to truncate the last two
lines of Eq. (5.4) into a single summation. As such,

\[
(FC)_{xy} = \sum_{\xi=\pm} \left( (\delta_{\xi,+} \pm \delta_{\xi,-}) |\bar{n}_f(0) - \bar{n}_f(\xi\bar{\omega})| \sum_{n=2}^{\infty} \frac{3n|\xi,n| \delta(\bar{\omega} - |\xi,n|)}{(|\xi,n|^2 + (4n-7)(4n-3)} \\
+ (\delta_{\xi,-} \pm \delta_{\xi,+}) |\bar{n}_f(0) - \bar{n}_f(\xi\bar{\omega})| \sum_{n=1}^{\infty} \frac{3(n-2)|\xi,n+1| \delta(\bar{\omega} - |\xi,n+1|)}{(4n-7)[(|\xi,n+1|^2 + (4n-3)]}
\right)

= 3 \sum_{\xi=\pm} (\delta_{\xi,+} \pm \delta_{\xi,-}) |\bar{n}_f(0) - \bar{n}_f(\xi\bar{\omega})| \sum_{n=0}^{\infty} \left( \frac{n+2}{4n+5} \pm \frac{n-1}{4n-3} \right) \frac{|\xi,n+2| \delta(\bar{\omega} - |\xi,n+2|)}{(\xi,n+2)^2 + 4n+1}

Next are the cone-cone transitions,

\[
(CC)_{xy} = \sum_{\xi, \xi'=\pm} (\delta_{\xi',-} \pm \delta_{\xi',+}) \sum_{n=2}^{\infty} \frac{|\bar{n}_f(\xi,n) - \bar{n}_f(\xi',n+1)|}{|\xi',n+1 - \xi,n|} \times f(\psi_{\xi',n+1}; \psi_{\xi,n})^2 \delta(\bar{\omega} - |\xi',n+1 - \xi,n|).
\]

The overlap function is

\[
|f(\psi_{\xi',n+1}; \psi_{\xi,n})|^2 = \frac{(n-1)|3\xi,n + \xi',n+1|^2}{[(\xi,n)^2 + 4n - 7][(|\xi',n+1|^2 + 4n - 3)].
\]

Thus,

\[
(CC)_{xx} = \sum_{\xi, \xi'=\pm} (\delta_{\xi',-} \pm \delta_{\xi',+}) \sum_{n=0}^{\infty} |\bar{n}_f(\xi,n+2) - \bar{n}_f(\xi',n+3)|
\times \frac{(n+1)|3\xi,n+2 + \xi',n+3|^2 \delta(\bar{\omega} - |\xi',n+3 - \xi,n+2|)}{|\xi',n+3 - \xi,n+2|[(\xi,n+2)^2 + 4n+1][(|\xi',n+3|^2 + 4n+5]}

= \frac{1}{4} \sum_{\xi, \xi'=\pm} (\delta_{\xi',-} \pm \delta_{\xi',+}) \sum_{n=0}^{\infty} |\bar{n}_f(\xi,n+2) - \bar{n}_f(\xi',n+3)|
\times \frac{(n+1)|6\xi' + |\xi',n+2|^{-1} + 9|\xi',n+3|^{-1} \delta(\bar{\omega} - |\xi',n+3 - \xi,n+2|)}{\sqrt{[(E_g/2)^2 + 4n+1][(|E_g/2|^2 + 4n+5]} |\xi',n+3 - \xi,n+2|}.
\]

(5.9)
Figure 5.2: Absorptive part of the longitudinal conductivity (black curve) for the 2D Kane system at zero temperature with $\mu = \gamma/2$ and $E_y = 0$. Contributions from sectors A and B are shaded red and blue, respectively.

**Sector B**

For sector B, the calculation follows the exact same procedure as in sector A. Using the spectrum of LL’s in Eq. (3.82), the contributions to the conductivity from sector B are

$$
(FC)_{xx} = \frac{3}{2} \sum_{\xi = \pm} (\delta_{\xi, +} \pm \delta_{\xi, -}) \sum_{n=0}^{\infty} \left| \bar{n}_f(0) - \bar{n}_f(\bar{\varepsilon}_{\xi, n+1}) \right|
$$

$$
\times \left( \frac{n + 2}{4n + 7} \pm \frac{n - 1}{4n - 1} \right) \frac{\delta(\bar{\omega} - \bar{\varepsilon}_{\xi, n+1})}{\sqrt{(E_g/2)^2 + 4n + 3}}
$$

(5.10)

$$
(CC)_{xx} = \frac{1}{4} \sum_{\xi' = \pm} (\delta_{\xi', -} \pm \delta_{\xi', +}) \sum_{n=0}^{\infty} \left| \bar{n}_f(\bar{\varepsilon}_{\xi, n+1}) - \bar{n}_f(\bar{\varepsilon}_{\xi', n+2}) \right|
$$

$$
\times \frac{(n + 1)|6\xi' + 9|\bar{\varepsilon}_{\xi, n+1}^{-1} + |\bar{\varepsilon}_{\xi', n+2}^{-1}| \delta(\bar{\omega} - |\bar{\varepsilon}_{\xi', n+2} - \bar{\varepsilon}_{\xi, n+1}|)}{\sqrt{[(E_g/2)^2 + 4n + 3][(E_g/2)^2 + 4n + 7]}} \frac{\bar{\varepsilon}_{\xi', n+2} - \bar{\varepsilon}_{\xi, n+1}}{\bar{\varepsilon}_{\xi', n+2} - \bar{\varepsilon}_{\xi, n+1}}.
$$

(5.11)
Analysis

The absorptive part of the zero-temperature longitudinal conductivity is plotted in Fig. 5.2 for $E_g = 0$ under a chemical potential $\mu \in (0, \gamma)$, which leaves the flat branch filled and the positive-energy branches empty. The delta functions have been replaced with Lorentzians (Eq. (4.8)) using a width of $\eta = 0.03$. The snowshoe diagrams corresponding to this spectrum are those found in Fig. 5.1. In the spectrum, the contribution from sector A is shaded red and that from sector B in blue. Each sector shows the same pattern in its series of peaks as the pseudospin-1 DW system, plotted in Fig. 4.7(a), whereby there is a non-monotonic decline in peak heights due to the second peak in each series. Rather than the contributions from each valley compounding, like the K and K' points in graphene and the dice lattice, the spectra from each sector in the Kane system are offset.

Seen in the next section, the spectrum in Fig. 5.2 relates well to the conductivity in 3D. The Lorentzian peaks are replaced by square-root singularities where the absorption edge lies at the exact energy as the 2D peak. The 3D regime also allows for inter-sector transitions since the disjoint chirality is broken.

5.2 3D Magneto-Optics

In 3D, LL’s are no longer single points in the Hilbert space, but 1D bands that disperse along $k_z$. Figure 5.3 plots this dispersion based on the LL energies in Eq. (3.83) for Kane fermions with $E_g = 0$.

The calculation of the conductivity tensor must now include a trace over $k_z$, making it possible for intra-sector transitions to occur ($\zeta = A \leftrightarrow B$),

$$
\sigma_{\alpha\beta}(\omega) = \frac{ig}{2\pi \hbar c_B^2} \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \sum_{\zeta,\zeta',n,n'} \sum_{\lambda,\lambda'} \frac{n_f(\epsilon_{\lambda,n}) - n_f(\epsilon_{\lambda',n'})}{\epsilon_{\lambda',n'}^\zeta - \epsilon_{\lambda,n}^\zeta} \frac{\langle \psi_{\lambda,n}^\zeta | j_\alpha | \psi_{\lambda',n'}^\zeta \rangle \langle \psi_{\lambda',n'}^\zeta | j_\beta | \psi_{\lambda,n}^\zeta \rangle}{\omega - (\epsilon_{\lambda',n'} - \epsilon_{\lambda,n}) + i\eta}.
$$

(5.12)
Figure 5.3: Landau level dispersion along $k_z$ in the Kane system. Sector A levels are coloured red and sector B in blue. At zero energy, there are numerous levels in both sectors, indicated by a purple band. The chemical potential, $\mu$ is marked with a green dashed line and arrows refer to transitions discussed in the text.
Applying the Kane model to this expression, the absorptive parts of the conductivity are

\[
\begin{align*}
\frac{\text{Re} \sigma_{xx}(\omega)}{\text{Im} \sigma_{xy}(\omega)} &= \frac{ge^2}{8\pi\hbar^2} \frac{\gamma}{v_0} \int_{-\infty}^{\infty} d\bar{k}_z \sum_{\lambda,\lambda',n,n'} \left[ \tilde{n}_f(\tilde{\varepsilon}_{\lambda,n}) - \tilde{n}_f(\tilde{\varepsilon}_{\lambda',n'}) \right] \delta(\tilde{\omega} - (\tilde{\varepsilon}_{\lambda',n'} - \tilde{\varepsilon}_{\lambda,n})) \\
&\quad \times \left( |f(\psi_{\lambda,n};\psi_{\lambda',n'})|^2 \delta_{n',n-1} \pm |f(\psi_{\lambda',n';\psi_{\lambda,n}})|^2 \delta_{n',n+1} \right),
\end{align*}
\]  

(5.13)

where we use \( \bar{k}_z = \hbar v_0 k_z / \gamma \) for brevity. The overlap function is now based on the six-element wavefunction and is the combination of the functions in Eq. (5.2),

\[
|f(\psi;\psi')|^2 = \left| \sqrt{3}\alpha_1 \alpha'_2 - \alpha_2 \alpha'_3 \pm \alpha_4 \alpha'_5 - \sqrt{3}\alpha_5 \alpha'_6 \right|^2.
\]  

(5.14)

Contributions to the conductivity can be categorized in two ways. The first uses the label \( \Phi_1 = \{AA, BB, AB\} \), where \( AA \) and \( BB \) refer to respective intra-sector transitions and \( AB \) to the set of inter-sector transitions. The other category uses the label \( \Phi_2 \),

\[
\begin{align*}
\cdot \Phi_2 &= 1: (\psi_{0,n} \leftrightarrow \psi_{\pm,n+1}) \text{ Transitions involving levels in the flat branch in which the zero-energy level is on the left (has the lower Fock number).} \\
\cdot \Phi_2 &= 2: (\psi_{\pm,n} \leftrightarrow \psi_{0,n+1}) \text{ Flat-branch transitions in which the zero-energy level is on the right (higher Fock number).} \\
\cdot \Phi_2 &= 3: (\psi_{\lambda \neq 0,n} \leftrightarrow \psi_{\lambda' \neq 0,n+1}) \text{ All transitions which do not involve the flat branch.}
\end{align*}
\]

The categorization \( (\Phi_1 \Phi_2) \) leads to nine separate sets of transitions. These are illustrated with snowshoe diagrams in the panels of Fig. 5.4. Note that due to the symmetry of the wavefunctions, the sector B state has the lower Fock number in all inter-sector transitions, \( (\psi_{\lambda,n}^B \leftrightarrow \psi_{\lambda',n+1}^A) \). The snowshoe diagrams are drawn at \( k_z = 0 \), but these transitions are allowed to disperse along the entire \( k_z \)-axis (subject to the Pauli exclusion principle). In fact, the intra-sector transitions indicated along the bottom row \( (\Phi_1 = AB) \) are prohibited from occurring at \( k_z = 0 \).
Figure 5.4: Snowshoe diagrams fixed at $k_z = 0$ showing the nine different sets ($\Phi_1 \Phi_2$), where the rows and columns are labelled $\Phi_1 = \{AA, BB, AB\}$ and $\Phi_2 = \{1, 2, 3\}$, respectively. Sector A levels are in red and sector B in blue. Branches not involved in a set are shaded grey.
The following derivation of the conductivity considers each of the sets in Fig. 5.4 separately,

\[
\begin{align*}
\text{Re} \sigma_{xx}(\omega) &= \frac{g e^2 \gamma}{8 \pi \hbar^2 v} \sum_{\Phi_1, \Phi_2} (\Phi_1 \Phi_2)_{xx} \cdot (\Phi_1 \Phi_2)_{xy} \cdot (\Phi_1 \Phi_2)_{yy}, \\
\text{Im} \sigma_{xy}(\omega) &= \text{ge}^2 \gamma \frac{8 \pi \hbar^2 v}{(\Phi_1 \Phi_2)_{xx} \cdot (\Phi_1 \Phi_2)_{xy} \cdot (\Phi_1 \Phi_2)_{yy}}.
\end{align*}
\]

(5.15)

The calculation uses the same procedure employed by Ashby and Carbotte used to determine the magneto-optical conductivity of the 3D \( s = 1/2 \) Weyl system [70].

**Contribution AA1**

Since the states involved in this part of the calculation all reside in sector A, the \( \zeta = A \) label is dropped. Right- and left-directed transitions are considered separately, but fit together nicely at the end of the calculation.

Beginning with the right-directed transitions \( (\psi_{0,n} \rightarrow \psi_{+,n+1}) \),

\[
(\text{AA1}_r)_{xx} = \pm \sum_{n=1}^{\infty} \frac{\bar{n}_f(0) - \bar{n}_f(\tilde{\omega})}{\tilde{\omega}} \int d\bar{k}_z \sum_{n=1}^{\infty} \left| f(\psi_{+,n+1}, \psi_{0,n}) \right|^2 \delta(g(\tilde{k}_z)),
\]

(5.16)

where

\[
g(\tilde{k}_z) = \tilde{\omega} - \tilde{E}_{g/2} - \sqrt{(\tilde{E}_{g/2})^2 + \tilde{k}_z^2 + 4n - 3}.
\]

(5.17)

The delta function can be simplified by the identity

\[
\delta(g(\tilde{k}_z)) = \sum_i \delta(\tilde{k}_z - \kappa_i),
\]

(5.18)

where \( \{\kappa_i\} \) is the set of all roots of \( g(\tilde{k}_z) \). Suppose \( \kappa_0 \) is one such root so that \( g(\kappa_0) = 0 \). Then

\[
\tilde{\omega} - \tilde{E}_{g/2} = \sqrt{(\tilde{E}_{g/2})^2 + \kappa_0^2 + 4n - 3} \quad \Longrightarrow \quad \tilde{\omega} - \tilde{E}_{g/2} > 0
\]

(5.19)

\[
\kappa_0^2 = \tilde{\omega}^2 - \tilde{E}_{g} \tilde{\omega} - (4n - 3).
\]

Note that the first line above requires that \( \tilde{\omega} > \tilde{E}_{g/2} \), otherwise the root does not exist.
Another requirement is that \( \kappa_0^2 > 0 \), leading to

\[
\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (4n - 3) > 0 \\
n < \frac{1}{4}(\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} + 3).
\] (5.20)

These extra considerations can be imposed by including a conditional factor on the integrand,

\[
\Theta(\tilde{\omega} - \tilde{E}_g/2) \Theta(\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (4n - 3)) .
\] (5.21)

Also,

\[
|g'(\kappa_0)| = \frac{|\kappa_0|}{\sqrt{(\tilde{E}_g/2)^2 + \kappa_0^2 + 4n - 3}} = \frac{\sqrt{\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (4n - 3)}}{\tilde{\omega} - \tilde{E}_g/2}.
\] (5.22)

Because the integrand is even in \( \bar{k}_z \), we need only consider the positive root, \( \kappa_0 > 0 \), accounting for the negative one by placing a factor of two on the identity in Eq. 5.18. Thus,

\[
\delta(g(\bar{k}_z)) = \frac{2(\tilde{\omega} - \tilde{E}_g/2)\delta(\bar{k}_z - \kappa_0)\Theta(\tilde{\omega} - \tilde{E}_g/2)\Theta(\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (4n + 3))}{\sqrt{\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (4n - 3)}}.
\] (5.23)

The necessary overlap functions are

\[
|f(\psi_{+,2}; \psi_{0,1})|^2|_{\bar{k}_z = \kappa_0} = \left( \frac{3(\tilde{\varepsilon}_{+,2})^2}{(\kappa_0^2 + 3)(\kappa_0^2 + 1 + (\tilde{\varepsilon}_{+,2})^2)} \right) \bigg|_{\bar{k}_z = \kappa_0} = \frac{3\tilde{\omega}}{2(\tilde{\omega} - \tilde{E}_g/2)(\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} + 2)},
\]

\[
|f(\psi_{+,n+1}; \psi_{0,n+3})|^2|_{\bar{k}_z = \kappa_0} = \left( \frac{3(n - 1)(n - 2)(\tilde{\varepsilon}_{+,n+1})^2}{(\kappa_0^2 + n - 1)(\kappa_0^2 + 4n - 7)(\kappa_0^2 + 4n - 3 + (\tilde{\varepsilon}_{+,n+1})^2)} \right) \bigg|_{\bar{k}_z = \kappa_0} = \frac{3(n - 1)(n - 2)\tilde{\omega}}{2(\tilde{\omega} - \tilde{E}_g/2)(\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - 4)[\tilde{\omega}^2 - \tilde{E}_g \tilde{\omega} - (3n - 2)]}.
\] (5.24)
Table 5.1: Arguments $x_1$ through $x_4$ of $\bar{N}_{f,\xi}(\Phi_2)$ in Eq. (5.28) for the different values of $\Phi_2$. Note that the $\Phi_2 = 3$ arguments are different for intra- and inter-sector transitions.

<table>
<thead>
<tr>
<th>$\Phi_2$</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$-\bar{\omega}$</td>
<td>0</td>
<td>0</td>
<td>$\bar{\omega}$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>$\bar{\omega}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3$_{\text{tra}}$</td>
<td>$\bar{E}_g/2 - \bar{\omega}^2/2 + \bar{E}_g/2$</td>
<td>$\bar{E}_g/2 - \omega^2 - \bar{E}_g/2$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3$_{\text{ter}}$</td>
<td>$\bar{E}_g/2 - \bar{\omega}^2/2 + \bar{E}_g/2$</td>
<td>$\bar{E}_g/2 - \omega^2 - \bar{E}_g/2$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Then

$$
(AA1_{r})_{xx} = \pm \left[ \bar{n}_f(0) - \bar{n}_f(\bar{\omega}) \right] \Theta(\bar{\omega} - \bar{E}_g/2) \left( \frac{3 \Theta(\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 - \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1}} \right)
$$

$$
+ \frac{3}{\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 4} \sum_{n=3} (n-1)(n-2) \left[ \frac{1}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 9)} \right] \frac{\Theta(\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 - \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1}}.
$$

$$
= \pm 3 \left[ \bar{n}_f(0) - \bar{n}_f(\bar{\omega}) \right] \Theta(\bar{\omega} - \bar{E}_g/2) \left( \frac{\Theta(\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 - \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 1}} \right)
$$

$$
+ \frac{1}{\bar{\omega}^2 - \bar{E}_g\bar{\omega} - 4} \sum_{n=0} (n+2)(n+1) \left[ \frac{1}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 9)} \right] \frac{\Theta(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1}}.
$$

(5.25)

The calculation for the left-directed transition follows the same procedure and produces a very similar form in the conductivity as the right-directed transitions

$$
(AA1_{l})_{xx} = 3 \left[ \bar{n}_f(-\bar{\omega}) - \bar{n}_f(0) \right] \Theta(-\bar{\omega} + \bar{E}_g/2) \left( \frac{\Theta(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1}} \right)
$$

$$
+ \frac{1}{\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 4} \sum_{n=0} (n+2)(n+1) \left[ \frac{1}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 9)} \right] \frac{\Theta(\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1)}{(\bar{\omega}^2 + \bar{E}_g\bar{\omega} + 2)\sqrt{\bar{\omega}^2 + \bar{E}_g\bar{\omega} - 1}}.
$$

(5.26)
The two results obtained in Eqs. (5.25) and (5.26) combine conveniently into a single expression for the set of AA1 transitions,

\[
(AA1)_{xx}^{xy} = 3 \sum_{\xi=\pm} N_{f,\xi}(1) \Theta(\bar{\omega} + \xi \bar{E}_g / 2) \left( \frac{\Theta(\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - 1)}{\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} + 2} \sqrt{\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - 1} \right) + \frac{1}{\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - 4} \sum_{n=0}^{\left\lfloor \frac{1}{4} \left( \bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - 9 \right) \right\rfloor} \frac{(n+2)(n+1)}{\left( \bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - (3n+7) \right) \sqrt{\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - (4n+9)}}.
\]

(5.27)

The joint distribution \( N_{f,\xi}(\Phi_2) \) is defined as

\[
N_{f,\xi}(\Phi_2) = [\bar{n}_f(x_1) - \bar{n}_f(x_2)] \delta_{\xi,+} \pm [\bar{n}_f(x_3) - \bar{n}_f(x_4)] \delta_{\xi,-},
\]

(5.28)

where the arguments \( x_1 \) through \( x_4 \) are listed in Table 5.1 for the different values that \( \Phi_2 \) takes. The object \( N_{f,\xi} \) contains the only distinction between longitudinal (\( xx \)) and transverse (\( xy \)) expressions.

At each value of \( \bar{\omega} \), the truncation on the sum in Eq. (5.27) stops \( n \) from being large enough to make the argument in the square root negative. If \( \bar{\omega} = \bar{\omega}_* \) is a value such that the cap on the sum is exactly an integer (so that the floor need not be applied), then the argument of the square root is exactly zero for the corresponding value of \( n \). This causes a divergence at \( \bar{\omega}_* \) in the form of a square-root singularity. This singularity, present for each transition, is due to a large resonance at \( \bar{k}_z = 0 \). As such, the singularities line up exactly with the delta peaks in the 2D spectrum. In Fig. 5.3, an example of this singular contribution is highlighted in orange, where a transition occurs from the flat branch into the first sector-A LL at \( \bar{k}_z = 0 \). As \( \bar{\omega} \) increases this transition can still be promoted, but at a higher \( \bar{k}_z \), leading to weaker contributions to the conductivity. This is indicated with the shrinking arrows in going from the singular transition to the right.
Contribution AA2

The contribution from the set $AA_2$ follows the same steps as in the other flat-branch set $AA_1$. It is a series of square-root singularities, placed at the same energies as in the other set ($AA_1$), but with different amplitudes. The result is

$$\langle AA_2 \rangle_{xx,xy} = 3 \sum_{\xi = \pm} \tilde{N}_f,\xi (2) \frac{\Theta (\bar{\omega} - \xi \bar{E}_g/2)}{\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega}} \frac{\frac{1}{2} (\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - 1)}{\sqrt{\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - (3n - 1)}}. \quad (5.29)$$

Contribution AA3

The cone-cone transitions are slightly more complicated to consider because neither state involved is fixed at zero energy. An explicit derivation requires separate consideration of four contributions, distinguishing between intra- and inter-cone as well as right- and left-directed transitions.

The right-directed intra-cone ($\psi_{+,n} \rightarrow \psi_{+,n+1}$) contribution is

$$\langle AA_{3++} \rangle_{xx,xy} = \int d\bar{k}_z \sum_{n=2}^{\infty} \frac{\tilde{n}_f (\bar{\varepsilon}_{+,n}) - \tilde{n}_f (\bar{\varepsilon}_{+,n+1})}{\bar{\omega}} |f(\psi_{+,n+1}; \psi_{+,n})|^2 \delta (g(\bar{k}_z)) \quad (5.30)$$

where now we have

$$g(\bar{k}_z) = \bar{\omega} + \sqrt{(\bar{E}_g/2)^2 + \bar{k}_z^2 + 4n - 7} - \sqrt{(\bar{E}_g/2)^2 + \bar{k}_z^2 + 4n - 3} \quad (5.31)$$

Suppose $g(\kappa_0) = 0$. Then,

$$\bar{\omega} = \sqrt{(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 3} - \sqrt{(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 7}$$

$$\bar{\omega}^2 = 2 \left[ (\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 5 - \sqrt{[(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 3][(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 7]} \right]$$

$$4\{\kappa_0^4 + 2[(\bar{E}_g/2)^2 + 4n - 5]\kappa_0^2 + [(\bar{E}_g/2)^2 + 4n - 5]^2\} - 4[(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 5]\bar{\omega}^2 + \bar{\omega}^4$$

$$= 4\{\kappa_0^4 + 2[(\bar{E}_g/2)^2 + 4n - 5]\kappa_0^2 + [(\bar{E}_g/2)^2 + 4n - 3][(\bar{E}_g/2)^2 + 4n - 7]\}$$

$$\kappa_0^2 = \frac{\bar{\omega}^4 - 4[(\bar{E}_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16}{4\bar{\omega}^2}. \quad (5.32)$$
At $\bar{k}_z^2 = \kappa_0^2$,

$$\bar{\varepsilon}_{+,n}|_{\kappa_0} = \frac{E_g}{2} + \frac{\sqrt{(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 7}}{2\bar{\omega}},$$

$$\bar{\varepsilon}_{+,n+1}|_{\kappa_0} = \frac{E_g}{2} + \frac{\sqrt{(\bar{E}_g/2)^2 + \kappa_0^2 + 4n - 7}}{2\bar{\omega}}.$$

(5.33)

But it must be that $\varepsilon_{+,n+1} - \varepsilon_{+,n} = \bar{\omega}$ (according to the delta function), requiring $\bar{\omega}^2 < 4$. In addition, the reality of $\kappa_0$ requires

$$\bar{\omega}^4 - 4[(\bar{E}_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16 > 0.$$  (5.34)

The roots of this polynomial are

$$\bar{\omega}_{\pm}^2 = 2 \left[ (\bar{E}_g/2)^2 + 4n - 5 \pm \sqrt{[(\bar{E}_g/2)^2 + 4n - 7][(\bar{E}_g/2)^2 + 4n - 3]} \right].$$  (5.35)

It is useful to note that both roots are positive and form the bounds of $\bar{\omega}^2 = 4$. That is,

$$0 < \bar{\omega}_-^2 < 4 < \bar{\omega}_+^2.$$  (5.36)

The proof of this statement comes in three parts (keeping in mind $n \geq 2$ here):

1. **Positivity:** Suppose $\bar{\omega}_-^2 > 0$. Then

$$\begin{align*}
(\bar{E}_g/2)^2 + 4n - 5 &> \sqrt{[(\bar{E}_g/2)^2 + 4n - 7][(\bar{E}_g/2)^2 + 4n - 3]} \\
&\implies (\bar{E}_g/2)^4 + 2(\bar{E}_g/2)^2(4n - 5) + 16n^2 - 40n + 25 \\
&> (\bar{E}_g/2)^4 + 2(\bar{E}_g/2)^2(4n - 5) + 16n^2 - 40n + 21 \\
&\implies 4 > 0,
\end{align*}$$

which is true.
2. **Lower Bound:** Suppose $\bar{\omega}^2 < 4$. Then

$$\bar{\omega}^2 < 4$$

$$\implies \sqrt{[(\bar{E}/2)^2 + 4n - 7][(\bar{E}/2)^2 + 4n - 3]} > (\bar{E}/2)^2 + 4n - 7$$

$$\implies (\bar{E}/2)^2 + 4n - 3 > \sqrt{(\bar{E}/2)^2 + 4n - 7},$$

which is true.

3. **Upper Bound:** Suppose $\bar{\omega}^2 > 4$. Then

$$\bar{\omega}^2 > 4$$

$$\implies - \sqrt{[(\bar{E}/2)^2 + 4n - 7][(\bar{E}/2)^2 + 4n - 3]} < (\bar{E}/2)^2 + 4n - 7,$$

which is true.

The inequality in Eq. (5.34) is satisfied for $\bar{\omega}^2 < \bar{\omega}_-^2$ and $\bar{\omega}^2 > \bar{\omega}_+^2$. However, the earlier requirement of $\bar{\omega}^2 < 4$ further restricts us to $\bar{\omega}^2 < \bar{\omega}_-^2$ only. This implies

$$2\sqrt{[(\bar{E}/2)^2 + 4n - 7][(\bar{E}/2)^2 + 4n - 3]} < 2[(\bar{E}/2)^2 + 4n - 5] - \bar{\omega}^2$$

$$\implies 4[(\bar{E}/2)^4 + 2(\bar{E}/2)^2(4n - 5) + (16n^2 - 40n + 21)]$$

$$< 4[(\bar{E}/2)^4 + 2(\bar{E}/2)^2(4n - 5) + (16n^2 - 40n + 25)]$$

$$+ \bar{\omega}^4 - 4[(\bar{E}/2)^2 + 4n - 5] \bar{\omega}^2$$

$$\implies n < \frac{\bar{\omega}^4 - 4[(\bar{E}/2)^2 - 5] \bar{\omega}^2 + 16}{16 \bar{\omega}^2}.$$  

This all lends to the conditional factor

$$\Theta(2 - \bar{\omega})\Theta\left(\bar{\omega}^4 - 4\left[(\bar{E}/2)^2 + 4n - 5\right] \bar{\omega}^2 + 16\right).$$  

(5.41)
Then, using the identity in Eq. (5.18),

\[
\delta(g'({\kappa_0})) = \frac{|g'({\kappa_0})|}{|{\kappa_0}|} \left| \frac{1}{\sqrt{{\kappa_0}^2 + (E_g/2)^2 + 4n - 3}} - \frac{1}{\sqrt{{\kappa_0}^2 + (E_g/2)^2 + 4n - 7}} \right| = \frac{\sqrt{\bar{\omega}^4 - 4[(E_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16} - \frac{2\bar{\omega}}{4 - \bar{\omega}^2 - \frac{2\bar{\omega}}{4 + \bar{\omega}^2}}}{2\bar{\omega}} \left| \right|_{(5.42)} = \frac{2\bar{\omega}^2}{16 - \bar{\omega}^4}\sqrt{\bar{\omega}^4 - 4[(E_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16}.
\]

Then, using the identity in Eq. (5.18),

\[
\delta(g(\bar{k}_z)) = \frac{(16 - \bar{\omega}^4)\Theta(2 - \bar{\omega})\Theta(\bar{\omega}^4 - 4[(E_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16)}{\bar{\omega}^2\sqrt{\bar{\omega}^4 - 4[(E_g/2)^2 + 4n - 5]\bar{\omega}^2 + 16}} \delta(\bar{k}_z - {\kappa_0}).
\]

The overlap function at \(\bar{k}_z = {\kappa_0}\) is

\[
(|f(\psi_{+,n+1}, \psi_{+,n})|^2)|_{\bar{k}_z = {\kappa_0}} = \left( \frac{(n - 1)|\bar{\epsilon}_{+,n} + \bar{\epsilon}_{+,n+1}|^2}{(k_z^2 + 4n - 7 + \bar{\epsilon}_{+,n}^2)(k_z^2 + 4n - 3 + \bar{\epsilon}_{+,n+1}^2)} \right)_{\bar{k}_z = {\kappa_0}} (5.44) = \frac{4\bar{\omega}^2(n - 1)(\bar{\omega}^2 - 2E_g\bar{\omega} - 8)^2}{(16 - \bar{\omega}^4)[(4 + E_g\bar{\omega})^2 - \bar{\omega}^4]}.
\]

This leads to the result

\[
(AA3_{++,})_{xy} = \pm\Theta(2 - \bar{\omega}) \left[ \bar{n}_f \left( \frac{\bar{E}_g/2 + 4 - \bar{\omega}^2}{2\bar{\omega}} \right) - \bar{n}_f \left( \frac{\bar{E}_g/2 + 4 + \bar{\omega}^2}{2\bar{\omega}} \right) \right] \times \frac{4(\bar{\omega}^2 - 2\bar{E}_g\bar{\omega} - 8)^2}{\bar{\omega}[(4 + E_g\bar{\omega})^2 - \bar{\omega}^4]} \sum_{n=2}^{16\bar{\omega}^2} \frac{n - 1}{\sqrt{\bar{\omega}^4 - 4[(E_g/2)^2 + 4n - 5] + 16}} (5.45) = \pm\Theta(2 - \bar{\omega}) \left[ \bar{n}_f \left( \frac{\bar{E}_g/2 + 4 - \bar{\omega}^2}{2\bar{\omega}} \right) - \bar{n}_f \left( \frac{\bar{E}_g/2 + 4 + \bar{\omega}^2}{2\bar{\omega}} \right) \right] \times \frac{4(\bar{\omega}^2 - 2\bar{E}_g\bar{\omega} - 8)^2}{\bar{\omega}[(4 + E_g\bar{\omega})^2 - \bar{\omega}^4]} \sum_{n=0}^{16\bar{\omega}^2} \frac{n + 1}{\sqrt{\bar{\omega}^4 - 4[(E_g/2)^2 + 4n + 3]\bar{\omega}^2 + 16}}.
\]

A similar calculation leads to the right-directed intra-cone \((\psi_{-,n+1} \rightarrow \psi_{-,n})\), AA3_{--}. 

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The left- and right-directed results gives the intra-cone contribution to the conductivity,

\[
(AA3_{+/---})_{xx} = \Theta(\tilde{\omega} - 2) \frac{4}{\bar{\omega}} \sum_{\xi = \pm} \tilde{N}_{f,\xi}(3_{\text{tra}}) (\tilde{\omega}^2 + 2\xi \tilde{E}_g \tilde{\omega} - 8)^2 \left( \frac{4 - \xi \tilde{E}_g \bar{\omega}}{(4 - \xi \tilde{E}_g \bar{\omega})^2 - \tilde{\omega}^4} \right) \left[ \frac{\omega^4 - (\tilde{E}_g^2 + 12) \bar{\omega}^2 + 16}{16\omega^2} \right] \times \sum_{n=0}^{\infty} \frac{n + 1}{\sqrt{\omega^4 - 4[(\tilde{E}_g/2)^2 + 4n + 3] \bar{\omega}^2 + 16}}.
\] (5.46)

In the result for the inter-cone pieces (\(\psi_{-/n} \rightarrow \psi_{+/n+1}\)) and (\(\psi_{-/n+1} \rightarrow \psi_{+/n}\)), all that differs from Eq. (5.46) is in the transformation of the factor

\[
\frac{\Theta(\bar{\omega} - 2)}{(4 - \xi \tilde{E}_g \bar{\omega})^2 - \bar{\omega}^4} \rightarrow \frac{\Theta(2 - \bar{\omega})}{\bar{\omega}^4 - (4 - \xi \tilde{E}_g \bar{\omega})^2}.
\] (5.47)

The sum of these two different factors is

\[
\frac{\Theta(2 - \bar{\omega}) - \Theta(\bar{\omega} - 2)}{\bar{\omega}^4 - (4 - \xi \tilde{E}_g \bar{\omega})^2} = \frac{1}{[\bar{\omega}^4 - (4 - \xi \tilde{E}_g \bar{\omega})^2]}.
\] (5.48)

Then the full \(AA3\) contribution is

\[
(AA3)_{xx} = \frac{4}{\bar{\omega}} \sum_{\xi = \pm} \tilde{N}_{f,\xi}(3_{\text{tra}}) (\tilde{\omega}^2 + 2\xi \tilde{E}_g \tilde{\omega} - 8)^2 \left( \frac{4 - \xi \tilde{E}_g \bar{\omega}}{(4 - \xi \tilde{E}_g \bar{\omega})^2 - \tilde{\omega}^4} \right) \left[ \frac{\omega^4 - (\tilde{E}_g^2 + 12) \bar{\omega}^2 + 16}{16\omega^2} \right] \times \sum_{n=0}^{\infty} \frac{n + 1}{\sqrt{\omega^4 - 4[(\tilde{E}_g/2)^2 + 4n + 3] \bar{\omega}^2 + 16}}.
\] (5.49)

Remaining Contributions

The remaining contributions each follow from similar derivations as those done above,

\[
(BB1)_{xx} = 3 \sum_{\xi = \pm} \tilde{N}_{f,\xi}(1) \Theta(\bar{\omega} + \xi \tilde{E}_g/2) \left( \frac{\Theta(\bar{\omega}^2 + \xi \tilde{E}_g \bar{\omega} - 3)}{\sqrt{\bar{\omega}^2 + \xi \tilde{E}_g \bar{\omega} - 3}} \right) + \frac{1}{\bar{\omega}^2 + \xi \tilde{E}_g \bar{\omega} - 4} \sum_{n=0}^{\infty} \frac{\left[ \frac{1}{2} \omega^2 + \xi \tilde{E}_g \bar{\omega} - (3n + 10) \right]}{\sqrt{\omega^2 + \xi \tilde{E}_g \bar{\omega} - (4n + 11)}}.
\] (5.50)
\[(BB2)_{xx \ y y} = 3 \sum_{\xi = \pm} \tilde{N}_{f, \xi}(2) \Theta(\bar{\omega} - \xi \bar{E}_g/2) \left( \frac{1}{4}(\omega^2 - \bar{E}_g \bar{\omega} - 3) \right) \sum_{n=0} (n+1)(n+2) \left[ \bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - (3n+2) \right] \sqrt{\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - (4n+3)} \right),

(5.51)\]

\[(BB3)_{xx \ y y} = \frac{4}{\bar{\omega}} \sum_{\xi = \pm} \tilde{N}_{f, \xi}(3_{\text{tra}}) \left( \frac{\bar{\omega}^2 - 2\xi \bar{E}_g \bar{\omega} + 8)^2}{\left[ \bar{\omega}^2 + (4 - \xi \bar{E}_g \bar{\omega})^2 \right]} \right) \left[ 4 \omega^2 - (\bar{E}_g^2 + 20) \omega^2 + 16 \right] \sum_{n=0} n + 1 \left( \bar{\omega}^2 - 4(\bar{E}_g/2)^2 + 4n+5 \right) \bar{\omega}^2 + 16 \right),

(5.52)\]

\[(AB1)_{xx \ y y} = 3 \sum_{\xi = \pm} \tilde{N}_{f, \xi}(1) \Theta(\bar{\omega} + \xi \bar{E}_g/2) \left[ \frac{1}{4}(\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - 5) \right] \sum_{n=0} (n+2) \sqrt{\bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - (4n+5)} \left( \bar{\omega}^2 + \xi \bar{E}_g \bar{\omega} - (3n+4) \right),

(5.53)\]

\[(AB2)_{xx \ y y} = 3 \sum_{\xi = \pm} \tilde{N}_{f, \xi}(2) \Theta(\bar{\omega} - \xi \bar{E}_g/2) \left[ \frac{1}{4}(\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - 7) \right] \sum_{n=0} (n+1) \sqrt{\bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - (4n+7)} \left( \bar{\omega}^2 - \xi \bar{E}_g \bar{\omega} - (3n+5) \right),

(5.54)\]

\[(AB3)_{xx \ y y} = \bar{\omega} \sum_{\xi = \pm} \tilde{N}_{f, \xi}(3_{\text{ter}}) \left[ \frac{1}{16}\omega^2 \left( \sqrt{\bar{\omega}^2 - 4(\bar{E}_g/2)^2 + 4n+2} \bar{\omega}^2 + 4 \right) \right] \sum_{n=0} \sqrt{\bar{\omega}^2 - (2 + \xi \bar{E}_g \bar{\omega})^2} \right),

(5.55)\]

All of the intra-sector contributions (AA and BB) are composed of a series of peaks made of square-root singularities. The absorption edge, the location of the singular part of the peak, occurs for a photon energy \(\bar{\omega}\) such that the argument on top of the summation is exactly an integer. At this value of \(\bar{\omega}\) and for \(n\) equal to the integer on top of the sum, the square root in the denominator of the summand is zero, causing the divergence. This behaviour comes from the \(\tilde{k}_z = 0\) part of the integration, where transitions resonate the most (orange transition in Fig. 5.3).

In the inter-sector contributions (AB), the square-root behaviour is instead in the numerator of the summand. As such, the peaks associated with these transitions are zero at the absorption edge. Recall that in 2D (i.e., when \(\tilde{k}_z\) is restricted to zero) there are no inter-sector transitions. Thus, there is no largely resonant transition at \(\tilde{k}_z = 0\) during the
Figure 5.5: Absorptive part of the longitudinal conductivity for the 3D Kane system at zero temperature with $E_g = 0$ and $\mu = \gamma/2$.

integration that would lead to a singular peak in the spectrum.

The absorptive part of the longitudinal conductivity (Re$\sigma_{xx}$ in Eq. (5.15)) at zero temperature and with $E_g = 0$ is plotted in Fig. 5.5. $\mu$ in the spectrum is such that all LL’s in flat branch are full and all positive-energy levels are empty (as in Fig. 5.3). At this value of $\mu$, there are no intra-branch transitions. The change in the spectrum with $\mu$ as different levels become partially filled or emptied follows the same logic behind changes in the $s = 1/2$ 3D Weyl spectrum. Because this has been detailed elsewhere [70], this aspect is not covered here.

Giving the parameter $E_g$ a finite value breaks particle-hole symmetry in the system. This affects the optical conductivity in minor ways. LL energies change with $E_g$, slightly shifting the location of peaks as long as $E_g$ remains small. There are many specific choices for parameters that one could discuss. However, of more concern here are the magneto-optics of the 3D Kane system in general, not for specific cases. In this broader discussion, we focus on a single simple selection of parameters ($k_B T = 0$, $E_g = 0$, and $\mu = \gamma/2$).

The main result of this piece of work is not the analysis of specific spectra, but rather the
Figure 5.6: Contributions from $\Phi_1 = AA$ transitions to $\text{Re} \sigma_{xx}$ in Fig. 5.5. $\Phi_2 = 1$ contributions are shaded red, $\Phi_2 = 2$ in blue, and $\Phi_2 = 3$ in green. The single green peak in the spectrum is indicated with an arrow.

Figure 5.7: Contributions from $\Phi_1 = BB$ transitions to $\text{Re} \sigma_{xx}$ in Fig. 5.5. Colouring is as in Fig. 5.6.
versatile analytic expressions above which can be used to model experiment at low energy and low magnetic field. This is relative to the range in energy for which the effective model applies.

To aid in the presentation of these results, the total conductivity in Fig. 5.5 is dissected into its three $\Phi_1$ contributions: $AA$ in Fig. 5.6, $BB$ in Fig. 5.7, and $AB$ in Fig. 5.8. Each of these latter figures breaks down the contributions further, showing $\Phi_2 = 1$ peaks in red, $\Phi_2 = 2$ in blue, and $\Phi_2 = 3$ in green. These colours are shown in transparency and mix when overlaid (red and blue make purple, etc.).

In Figs. 5.6 and 5.7, the absorption edge of each singular peak lies at the same location as the corresponding Lorentzian peak in the 2D conductivity found in Fig. 5.2. This large resonance comes from the $\vec{k}_z = 0$ contribution in the transition between the 1D LL’s that stretch along the $\vec{k}_z$-axis. As $\vec{k}_z$ is traced out away from the origin the energy separation between LL’s steadily increases. This leads to the tails on each singular peak in the 3D spectrum that trail off to higher energy. These tails build on each other to give an overall linear trend, as is expected for the conductivity of a 3D relativistic system [71].

Figure 5.8: Contributions from $\Phi_1 = AB$ transitions to $\text{Re}\sigma_{xx}$ in Fig. 5.5. Colouring is as in Fig. 5.6.
Figure 5.9: Transverse optical conductivity in the zero-temperature 3D Kane system with $E_g = 0$ and $\mu = \gamma/2$. Indicated is a dip below zero in the spectrum that is discussed in the text.

Suppose that the value of $\mu$ was such that an intra-branch transition was allowed, like $(\psi_{+, n} \rightarrow \psi_{+, n+1})$. Again, the singular contribution comes from the transition at $\vec{k}_z = 0$. Unlike the transitions contributing to Fig. 5.5, the separation between two LL’s with the same sign is largest at $\vec{k}_z = 0$. As $\vec{k}_z$ is traced away from the origin, the separation decreases, which would lead to a tail on the associated peak that trails off to lower energy.

In each of the intra-sector plots (Figs. 5.6 and 5.7), the flat-branch transitions (blue and red) dominate over the cone-cone transitions (green). This is the same as in the 2D Kane and $s = 1$ DW systems. In the DW systems, transitions with $\Delta \lambda > 1$ are largely surpressed. The Kane system shares this trait, as it is closely related to the three-band $s = 1$ DW system (demonstrated via the mapping of the Kane model onto the $\alpha$-$T_3$ model). The single inter-branch transition in each plot is indicated with an arrow. The green peak in the $AA$ spectrum occurs at a lower energy than in the $BB$ spectrum, yet is smaller in height (contrary to the general trend of larger peaks at lower energy). This is because the $BB$ peak arises from a transition involving a lower Fock number $n$, which also has bearing
Figure 5.10: Optical conductivity for right-handed polarized light in the zero-temperature 3D Kane system with $E_g = 0$ and $\mu = \gamma/2$. An arrow indicates a peak that is discussed in the text.

In Fig. 5.10, the inter-sector contributions ($AB$) present as peaks with a regular square-root profile, each of which is zero at the absorption edge. The total spectral weight of these $AB$ transitions is quite small and cannot be discerned from the full conductivity in Fig. 5.5.

The transverse conductivity, $\text{Im} \sigma_{xy}$, is plotted in Fig. 5.9 under the same parameters that have been used thus far ($k_B T = 0$, $E_g = 0$, and $\mu = \gamma/2$). Positive regions of the spectrum are dominated by right-directed transitions and negative by the left-directed ones. Around the energy $\bar{\omega} \sim 2.5$, the spectrum dips slightly below zero. This negative dip is due to the presence of inter-sector transitions. If the $AB$ transitions are not included in the calculation of $\text{Im} \sigma_{xy}$, this region is positive. Thus, unlike $\text{Re} \sigma_{xx}$, this spectrum provides an indication of the occurrence of inter-sector transitions.

Finally, optical conductivity for the two circular polarizations of light are given in Figs. 5.10 and 5.11, showing $\text{Re} \sigma_+$ and $\text{Re} \sigma_-$, respectively. In the same spectra for the $s = 1$ DW system, Figs. 4.9(a) and 4.10(a), the second peak seen in the left-handed spectrum
Figure 5.11: Optical conductivity for left-handed polarized light in the zero-temperature 3D Kane system with $E_g = 0$ and $\mu = \gamma/2$. An arrow indicates a peak that is discussed in the text.

is absent from the right-handed spectrum. This is a result of there being no right-directed transition from the flat branch into a particular positive-energy LL. This same effect happens in both the $AA$ and $BB$ sets of transitions. Each set produces a series of sharp peaks in which the second peak in a set is absent from the right-handed spectrum. The second peak in the $AA$ series is indicated with an arrow in Fig. 5.11. The peak to its right is the second peak in the $BB$ series. Both of these sharp peaks are absent from the other spectrum (Fig. 5.10), revealing intra-sector transitions in their place. Then, contributions from the intra- and inter-sector transitions which terminate on the states $\psi^A_{+,3}$ and $\psi^B_{+,2}$ can be separated out by using circularly polarized light.

The analytic expressions in Eqs. (5.27), (5.29), and (5.49)-(5.55) are the main result of this section. Armed with fully analytic expressions and their step-by-step derivation, many details in optical spectra and their origins become evident. Also, these expressions may be used to model the magneto-optical properties of physical systems at low energy described by the Kane model.
5.3 MCT Magneto-Optics

The general Kane model in Eq. (3.74) applies to small-gap zincblende structures in which it is sufficient to approximate the heavy-hole band as flat. One such material is Hg$_{1-x}$Cd$_x$Te (MCT). For a Cd:Te ratio of $x = x_c \sim 0.17$, the gap $E_g$ (and effective quasiparticle mass) has been known for decades to be very small [72]. Modern interest in Dirac materials and linearized band structure motivated Orlita et al. to perform a series of optical measurements on MCT at this critical ratio, $x_c$ [29]. They confirmed the relativistic nature of this phase of the material through observation of a linear energy dependence in the zero field optical conductivity and a $\sqrt{B}$ dependence in the location of peaks in the magneto-optics. The quasiparticle excitations therein were coined as massless Kane fermions. In this section, the frequency-dependent experimental data from the optical measurements on MCT is modelled for both zero-field and $B = 16$ T.

In order to more accurately model physical MCT, the $\Delta \to \infty$ approximation is not sufficient. Instead, the value $\Delta = 1$ eV is used, along with $E_g = 4$ meV and $v = 1.01 \times 10^6$ m/s, in order to match the experimental parameters. By including a finite $\Delta$ into the model, the optical conductivity can no longer be solved analytically. More specifically, explicit expressions cannot be found for the eigensystem of Eq. (3.74).

At zero magnetic field, the absorptive part of the longitudinal conductivity is

$$\text{Re } \sigma_{xx}(\omega) = \frac{1}{8\pi \hbar} \int d^3k \sum_{\psi, \psi'} \frac{n_f(\varepsilon) - n_f(\varepsilon')}{\varepsilon' - \varepsilon} |\langle \psi | \hat{j}_x | \psi' \rangle|^2 \delta(\omega - (\varepsilon' - \varepsilon)) ,$$  \hspace{1cm} (5.56)

where the summation on $\psi$ is over the two sectors in the model with four bands each. For the energy scale considered in the following analysis, it is not necessary to include transitions from the $\Delta$ band. This fourth band is located below the others, separated by $\Delta = 1$ eV. While it does not contribute directly to the conductivity, its inclusion in the model is necessary because of the curvature it induces in the remaining band structure.

In order to compute Eq. (5.56) numerically, a code was written in Python that evaluated the integral above for different values of $\omega$, using a Lorentzian peak (Eq. (4.8)) with a width of $\eta = 2$ meV. At each point $k$ the eigensystem of Eq. (3.74) was determined numerically.
Figure 5.12: Absorption coefficient from the Kane model for two different values of $\Delta$ (solid red and dashed blue) against an experimental measurement of MCT [29]. Inset is a cross section of the band structure for the two different $\Delta$, with an illustration of an optical transition.

The Hamiltonian does not depend on the azimuthal angle $\tan \varphi = k_y/k_x$, which allows for the reduction in costly integration variables,

$$
\int d^3k \rightarrow 2\pi \int_{-\infty}^{\infty} dk_z \int_{0}^{\infty} dk_{\perp} k_{\perp}, \quad k_{\perp} = \sqrt{k_x^2 + k_y^2}.
$$

The result of the numerical integration by the Euler method is presented in Fig. 5.12 as the absorption coefficient (red curve), $\lambda(\omega) = \sqrt{4\omega \sigma/\epsilon_0 \hbar c^2}$ (note that $\Omega$ is used in place of $\omega$ in the figure). The blue curve in the figure is the same but for $\Delta \rightarrow \infty$. Inset is a cross section of the band structure for these two regimes, showing a clear curvature in the cones for the finite-$\Delta$ case. The black curve in the figure is taken from experiment. The experimental curve is not plotted for energy below about 40 meV as it is dominated by a large phonon peak and the Restrahlen band [29]. The vertical offset between experiment and theory is due a small mismatch in the dielectrics of the MCT and its substrate that was not accounted for. At low energy the two theoretical curves largely agree. However,
as energy grows, it becomes clear that it is necessary to consider the finite Δ in order to accurately model MCT. The difference becomes appreciable around 150 or 200 meV.

In the presence of a magnetic field in the z-direction, the $k_x$ and $k_y$ momentum operators transform into Fock operators, $k_+ \rightarrow \sqrt{2a^\dagger/\ell_B}$ ($k_- \rightarrow \sqrt{2a/\ell_B}$). The general form of the wavefunction involves a Fock state in each element of the 8-spinor upon which these operators act,

$$\psi = (\alpha_1|n-3\rangle, \alpha_2|n-2\rangle, \alpha_3|n-1\rangle, \alpha_4|n-1\rangle, \alpha_5|n-2\rangle, \alpha_6|n-2\rangle, \alpha_7|n-1\rangle, \alpha_8|n\rangle)^T.$$  (5.58)

The abstract Fock space is difficult to handle in the numerics, so the action of the Fock operators is made explicit, where

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \ a|n\rangle = \sqrt{n}|n-1\rangle.$$  (5.59)

A Fock state cannot be labelled with a negative number $n$. To deal with this feature, a new square root operator is defined which is non-zero only for positive values in its argument,

$$\sqrt[\gamma]{x} \equiv \sqrt{\Theta(x)}.$$  (5.60)

The Hamiltonian now becomes

$$\hat{H} = \gamma \left( \begin{array}{cc} \hat{A} & \hat{C} \\ \hat{C}^T & \hat{B} \end{array} \right),$$  (5.61)

where

$$\hat{A} = \begin{pmatrix} 0 & \sqrt{3(n-2)} & 0 & 0 \\ \sqrt{3(n-2)} & E_g & -\sqrt{n-1} & -\sqrt{2(n-1)} \\ 0 & -\sqrt{n-1} & 0 & 0 \\ 0 & -\sqrt{2(n-1)} & 0 & -\Delta \end{pmatrix},$$  (5.62)
\[
\hat{B} = \begin{pmatrix}
-\bar{\Delta} & 0 & -\sqrt[2]{2(n-1)} & 0 \\
0 & 0 & \sqrt{n-1} & 0 \\
-\sqrt[2]{2(n-1)} & \sqrt{n-1} & \bar{E}_g & -\sqrt[3]{3n} \\
0 & 0 & -\sqrt[3]{3n} & 0 
\end{pmatrix}, \tag{5.63}
\]

\[
\hat{C} = \begin{pmatrix}
0 & 0 & 0 & 0 \\
-\bar{k}_z & 0 & 0 & 0 \\
0 & -\bar{k}_z & 0 & 0 \\
0 & 0 & -\frac{\bar{k}_z}{\sqrt{2}} & 0
\end{pmatrix}. \tag{5.64}
\]

The LL energy spectrum for \( B = 16 \) T, determined numerically, is shown in Fig. 5.13. Based on the symmetry of the wavefunctions in Eq. (3.84) (i.e., observing which elements are always zero), it is possible to sort the computer-generated wavefunctions into sectors A and B. In the figure, sector A LL’s are drawn with solid red lines and sector B LL’s with dashed blue lines. There are many LL’s from either sector at zero energy, marked with a thick green band.

The magneto-optical conductivity follows from Eq. (5.12). In setting up the computation, snowshoe diagrams like in Fig. 5.4 are helpful in making sense of the web of possible transitions between LL’s. This is especially true for \( n < 3 \) where the physically viable state space is restricted (based on Eq. (5.58)). The diagonalization routine used to find the eigensystem of Eq. (5.61) has difficulties with the zero-energy LL’s (and their double degeneracy for \( n \geq 3 \)). Luckily, the wavefunctions for these states, \( \psi^\xi_{0,n} \), can be determined analytically,

\[
\psi^A_{0,1} = \kappa(0, 0, \sqrt{3}, 0, 0, 0, 0, -\bar{k}_z)^T, \\
\psi^A_{0,n \geq 3} = \kappa(\bar{k}_z^2 + n - 1, 0, \sqrt{3(n-1)(n-2)}, 0, 0, \sqrt{3(n-1)(n-2)}k_z, 0, 0)^T, \tag{5.65}
\]

\[
\psi^B_{0,0} = (0, 0, 0, 0, 0, 0, 0, 1)^T, \\
\psi^B_{0,n \geq 2} = \kappa(0, 0, -\sqrt{3nk}_z, 0, 0, \sqrt{3n(n-1)}, 0, \bar{k}_z^2 + n - 1)^T.
\]

In Fig. 5.14(b), the resulting numerical integration is used to plot the absorbance spectrum, \( A = \lambda d \), for a sample thickness of \( d = 3.2 \) µm. The calculation (red) shows good
agreement to the experimental measurement (black), with a vertical offset as in Fig. 5.12 explained by the substrate dielectric mismatch. In the top panel of the figure, the optical conductivity is plotted for the system restricted to 2D, showing Lorentzian peaks which line up with the absorption edges of peaks in the bottom panel. Indicated with black arrows are those reduced-height second peaks which act as indicators of the presence of a flat band.

At an energy of about 100 meV, the experimental spectrum in Fig. 5.14(b) shows a small shoulder built on the first peak (red arrow). This feature was drawn out in the theoretical curve by slightly filling the lowest positive LL, $\psi_{+,2}^A$. This allows for a small number of intra-branch transitions to occur ($\psi_{+,2}^A \rightarrow \psi_{+,3}^A$, red arrow in Fig. 5.13) building up this small shoulder. This is referred to as the cyclotron resonance peak in the quantum limit (this limit being where positive-energy fermions are pushed into the lowest-lying LL). As this shoulder grows, the height of the first peak is reduced since a portion of the LL $\psi_{+,2}^A$ is locked out of being involved in a transition from the flat branch. The degree of filling of this LL was determined phenomenologically in order to best match the size of the shoulder.
Figure 5.14: (a) Absorptive part of the longitudinal conductivity for the Kane model in a magnetic field ($B = 16$ T) restricted to 2D. Sector A transitions are coloured red and sector B in blue. (b) Theoretical (red) and experimental (black) absorbance of 3D MCT in a magnetic field. In both panels, arrow indicate peaks discussed in the text.
in the experimental curve. This was achieved by filling the LL in a small region \( k_z \in (-q, q) \) and extending \( q \) until a suitable result was obtained.

Calculating the MCT optical spectra in Figs. 5.12 and 5.14 extends the large body of work done on this material by Orlita et al. [29,31]. By computing the frequency-dependent conductivity using the Kane model, not only are peak locations confirmed, but also the spectral weight of each peak. The success of the linearized Kane model in describing MCT’s physical properties lends to the strength in identifying this as a relativistic material where the heavy hole band may be treated as flat. MCT is a material with both pseudospin-1/2 and pseudospin-1 character (because of the relationship between the Kane and \( \alpha-T_3 \) models). The existence of materials in nature which show at least some pseudospin-1 character motivates further investigations into the properties of the pure higher-pseudospin systems.
Chapter 6

Pseudospin-1 Polarizability

In this chapter, the dynamical polarizability function of the $s = 1$ DW system is derived (in the absence of any magnetic field). Prior to the derivation, this function for the $s = 1/2$ system is presented in order to make subsequent comparisons. The main difference between the two systems is that the former is host to a singular density of states in the form of a flat band at zero energy. The flat band has ramifications on the polarizability function and on the collective behaviour of charge carriers in the $s = 1$ system.

It was shown in Chapter 3 that the dice lattice gives rise to $s = 1$ DW fermions in its low energy dynamics. As such, ‘$s = 1$’ and ‘the dice lattice’ are used interchangeably to refer to the system under study. However, despite the specific references to the dice lattice throughout this chapter, the analysis applies to all $s = 1$ DW systems. The same goes for ‘graphene’ being used to refer to the $s = 1/2$ DW system.

Because the DW system is particle-hole symmetric and because the polarization function has the identity $Q^*(\omega) = Q(-\omega)$, we restrict the derivation to $\mu > 0$ and $\omega > 0$ without loss of generality. For brevity, units are chosen such that $\hbar = v = 1$, where $v$ is the Fermi velocity in the conic band.

The original results and many of the figures presented in this chapter have been published in Ref. [73].

6.1 Graphene Polarizability

In the context of graphene, the $s = 1/2$ polarizability function has been derived many times, including with extra considerations such as a finite gap or a sublattice potential
Figure 6.1: Imaginary part of the graphene polarizability function. White regions mark the void in the particle-hole continuum (where $\text{Im} \ Q = 0$).

Figure 6.2: Real part of the graphene polarizability function.
difference [74–79]. In this section, the graphene polarizability in the RPA is presented for zero temperature and a variable $\mu$. This is done for comparison with the dice polarizability derived later.

First, the imaginary part of the graphene polarizability is

$$\text{Im} \frac{Q(q, \omega)}{16\pi}$$

$$= \Theta(q - \omega) \Theta(2\mu + \omega - q)$$

$$\times \left[ (2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{q^2 - \omega^2}} + \frac{q^2}{\sqrt{q^2 - \omega^2}} \ln \left| \frac{q}{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}} \right| \right]$$

$$+ \Theta(q - \omega) \Theta(2\mu - \omega - q)$$

$$\times \left[ -(2\mu - \omega) \sqrt{\frac{(2\mu - \omega)^2 - q^2}{q^2 - \omega^2}} - \frac{q^2}{\sqrt{q^2 - \omega^2}} \ln \left| \frac{q}{2\mu - \omega + \sqrt{(2\mu - \omega)^2 - q^2}} \right| \right]$$

$$+ \Theta(\omega - q) \Theta(q - |2\mu - \omega|)$$

$$\times \left[ -(2\mu - \omega) \sqrt{\frac{q^2 - (2\mu - \omega)^2}{\omega^2 - q^2}} + \frac{q^2}{\sqrt{\omega^2 - q^2}} \arccos \left( \frac{2\mu - \omega}{q} \right) \right]$$

$$+ \Theta(\omega - q - 2\mu) \left[ \frac{\pi q^2}{\sqrt{q^2 - \omega^2}} \right] .$$

(6.1)
The Kramers-Kronig related real part is

\[ \text{Re} \frac{Q(q, \omega)}{16\pi} = 8\mu \]

\[ + \Theta(q - \omega) \Theta(\omega + q - 2\mu) \times \left[ -(2\mu - \omega) \sqrt{\frac{q^2 - (2\mu - \omega)^2}{q^2 - \omega^2}} + \frac{q^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu - \omega}{q} \right) \right] \]

\[ + \Theta(q - \omega - 2\mu) \times \left[ -(2\mu + \omega) \sqrt{\frac{q^2 - (2\mu + \omega)^2}{q^2 - \omega^2}} + \frac{q^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu + \omega}{q} \right) \right] \]

\[ + \Theta(\omega - q) \Theta(|2\mu - \omega| - q) \times \left[ |2\mu - \omega| \sqrt{\frac{(2\mu - \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{q^2}{\sqrt{\omega^2 - q^2}} \ln \left| 2\mu - \omega + \sqrt{(2\mu - \omega)^2 - q^2} \right| \right] \]

\[ + \Theta(\omega - q) \times \left[ -(2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{q^2}{\sqrt{\omega^2 - q^2}} \ln \left| 2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2} \right| \right]. \]

These objects are plotted separately as colour maps in Figs. 6.1 and 6.2.

With \( \text{Im} Q \) being an on-shell quantity, the non-zero region in \((q, \omega)\)-space is referred to as the particle-hole continuum (PHC). This continuum highlights areas where it is possible to make a geometric connection between a filled state and empty state which are separated by a momentum \( q \) and energy \( \omega \). White regions in Fig. 6.1 mark the void in the PHC, where \( \text{Im} Q = 0 \). The diagonal stripe in the PHC, characterized by the boundaries \( \omega < q < 2\mu + \omega \), comes from intracone contributions. This region exhibits the scattering events of a particle from a state in the upper cone, below the Fermi level, being scattered into a hole state \( (s = 1/2 \text{ in Fig. 3.1}) \). The other part of the graphene PHC, where \( \omega > q \), comes from inter-cone scattering (lower to upper cone).
6.2 Dice Polarizability

From Eq. (2.51), the general formula for the polarizability in a 2D system (in the absence of a magnetic field) is

$$Q(q, \omega) = \frac{g}{4\pi^2} \int d^2k \sum_{\lambda, \lambda'} \frac{n_f(\varepsilon_{\lambda'}(k')) - n_f(\varepsilon_{\lambda}(k))}{\omega - (\varepsilon_{\lambda'}(k') - \varepsilon_{\lambda}(k)) + i\eta} F_{\lambda\lambda'}(k),$$

(6.3)

where $k' = k + q$ and the scattering amplitude is

$$F_{\lambda\lambda'}(k) = |\langle \psi_{\lambda}(k)|\psi_{\lambda'}(k') \rangle|^2.$$ (6.4)

The dice lattice at low energy has three energy bands, $\varepsilon_{\lambda}(k) = \lambda k$, which are linear in momentum, $k = (k, \theta)$, and labelled by the indices $\lambda = \{0, \pm 1\}$. At zero temperature and for $\mu > 0$, the distribution functions become

$$n_f(\varepsilon_-) = n_f(\varepsilon_0) = 1, \quad n_f(\varepsilon_+) = \Theta(\mu - k).$$ (6.5)

Then the only non-zero contributions to the sum in Eq. (6.3) will have either or both of $\lambda$ or $\lambda'$ equal to +1, making it only necessary to compute the scattering amplitudes $F_{+\lambda} = F_{\lambda+}$.

The wavefunctions for single-particle states in each band are

$$\psi_0(k) = \frac{1}{\sqrt{2}} (1, 0, e^{i2\theta} )^T, \quad \psi_{\pm}(k) = \frac{1}{2} (1, \pm \sqrt{2} e^{i\theta}, e^{i2\theta})^T.$$ (6.6)

The inner product of two wavefunctions at different locations in reciprocal space will involve the angle between $k$ and $k'$, $\varphi_k = \theta - \theta'$, where

$$\cos \varphi_k = \frac{k \cdot k'}{kk'} = \frac{k + q \cos \theta}{\sqrt{k^2 + q^2 + 2qk \cos \theta}}.$$ (6.7)
The relevant scattering amplitudes are

\[
F_{+0}(k) = \frac{1}{8} \left| 1 - e^{i2\varphi_k} \right|^2 = \frac{1}{8} \left| e^{-i\varphi_k} - e^{i\varphi_k} \right|^2 = \frac{1}{2} \sin^2 \varphi_k ,
\]

(6.8)

\[
F_{++}(k) = \frac{1}{16} \left| 1 + 2e^{i\varphi_k} + e^{2i\varphi_k} \right|^2 = \frac{1}{16} \left| e^{-i\varphi_k} + e^{i\varphi_k} \pm 2 \right|^2 = \frac{1}{4} (\cos \varphi_k \pm 1)^2 .
\]

(6.9)

**Imaginary Part**

The imaginary part of the polarizability in Eq. (6.3) is

\[
\text{Im} Q(q, \omega) = \frac{g}{4\pi} \int d^2k \sum_{\lambda, \lambda'} \left[ n_f(\varepsilon_\lambda(k)) - n_f(\varepsilon_{\lambda'}(k')) \right] \delta(\omega - (\varepsilon_{\lambda'}(k') - \varepsilon_{\lambda}(k))) F_{\lambda\lambda'}(k) .
\]

(6.10)

By excluding terms with a non-zero argument of the delta function for all \( k > 0 \) (such as \( \delta(\omega + k) \)), and making use of the symmetry \( k \to k' \) and the identity

\[
1 - \Theta(x) = \Theta(-x) ,
\]

(6.11)

then Eq. (6.10) can be split into four terms,

\[
\text{Im} Q = \sum_{j=1}^4 I_j ,
\]

(6.12)
where

\[ I_1 = \frac{g}{4\pi} \int d^2k \Theta(\mu - k)\delta(\omega - (k' - k)) F_{++}(k), \]

\[ I_2 = -\frac{g}{4\pi} \int d^2k \Theta(\mu - k)\delta(\omega - (k - k')) F_{++}(k), \]

\[ I_3 = \frac{g}{4\pi} \int d^2k \Theta(k - \mu)\delta(\omega - (k' + k)) F_{+-}(k), \]

\[ I_4 = \frac{g}{4\pi} \int d^2k \Theta(k - \mu)\delta(\omega - k) F_{+0}(k), \]

(6.13)

The term \( I_4 \) is the contribution due to scattering from the flat band, an effect that is absent from the graphene polarizability.

Starting with \( I_1 \), we employ the identity in Eq. (5.18) to evaluate the integral over \( d\theta \),

\[ \delta(g(\theta)) = \frac{2\delta(\theta - \theta_0)}{|g'(\theta_0)|}, \]

(6.14)

where \( \theta_0 \) is the root of \( g(\theta) \) along the semi-circle \( \theta \in (0, \pi) \). If the root \( \theta_0 \) exists, then, because the only \( \theta \)-dependence in the integrand is found in \( \cos \theta \), there will also be a root on \( \theta \in (-\pi, 0) \). This second root is accounted for by the factor of two in Eq. (6.14). No further considerations of the second root need to be taken since the integrand is even about \( \theta = 0 \).

With \( g(\theta) = \omega - (k' - k) \), suppose \( g(\theta_0) = 0 \). Then

\[ \omega + k = \sqrt{k^2 + q^2 + 2qk \cos \theta_0} \]

\[ \cos \theta_0 = \frac{2\omega k + \omega^2 - q^2}{2qk}. \]

(6.15)

The existence of the root requires \( \cos^2 \theta_0 < 1 \), or

\[ (q^2 - \omega^2)[(2k + \omega)^2 - q^2] > 0. \]

(6.16)

The polynomial in the inequality of Eq. (6.16) has the roots \( k_\pm = (-\omega \pm q)/2 \). Two cases arise,

1. \( q > \omega \) (which means \( k_- < 0 < k_+ \)). The inequality above is satisfied when the
polynomial is positive, or when \( k > k_+ \).

2. \( q < \omega \) (which means \( k_+ < 0 \)). Here the polynomial must be negative, which does not occur for any \( k > 0 \). As such, this case is rejected (no root of \( g(\theta) \) exists here).

With these considerations, a conditional factor is included,

\[
\Theta(q - \omega)\Theta(2k + \omega - q).
\] (6.17)

Further,

\[
|g'(\theta_0)| = \frac{qk|\sin \theta_0|}{\sqrt{k^2 + q^2 + 2qk \cos \theta_0}}.
\] (6.18)

Well, we have

\[
|\sin \theta_0| = \sqrt{1 - \cos^2 \theta_0} = \frac{\sqrt{(q^2 - \omega^2)(2k + \omega)^2 - q^2}}{2qk},
\] (6.19)

so that

\[
|g(\theta_0)| = \frac{\sqrt{(q^2 - \omega^2)(2k + \omega)^2 - q^2}}{2(\omega + k)}.
\] (6.20)

Then the delta function is replaced by the expression

\[
\delta(g(\theta)) = \frac{4(\omega + k)\delta(\theta - \theta_0)}{\sqrt{(q^2 - \omega^2)(2k + \omega)^2 - q^2}}\Theta(q - \omega)\Theta(2k + \omega - q).
\] (6.21)

Calling \( k_0 = (k, \theta_0) \), we require

\[
\cos \varphi_{k_0} = \frac{k + q \cos \theta_0}{\sqrt{k^2 + q^2 + 2qk \cos \theta_0}} = \frac{2k^2 + 2\omega k + \omega^2 - q^2}{2k(\omega + k)}.
\] (6.22)

Then

\[
F_{++}(k_0) = \frac{1}{2}(1 - \cos^2 \varphi_{k_0}) = \frac{[(2k + \omega)^2 - q^2]^2}{16k^2(\omega + k)^2}.
\] (6.23)
Thus, tracing out $d\theta$ in $I_1$ gives

$$I_1 = \frac{g}{16\pi} \frac{\Theta(q - \omega)}{\sqrt{q^2 - \omega^2}} \int_0^\mu dk \frac{\Theta(2k + \omega - q) [(2k + \omega)^2 - q^2]^{3/2}}{k(k + \omega)}.$$  \hspace{1cm} (6.24)

The final result for $I_1$ proceeds via the integration over $dk$, which at one point involves a change of dummy variables to $x = 2k + \omega$,

$$I_1 = \frac{g}{16\pi} \frac{\Theta(q - \omega) \Theta(2\mu + \omega - q)}{\sqrt{q^2 - \omega^2}} \int_{x=q}^\mu \frac{dk}{k(k + \omega)} \frac{[(2k + \omega)^2 - q^2]^{3/2}}{k(k + \omega)}$$

$$= \frac{g}{16\pi} \frac{\Theta(q - \omega) \Theta(2\mu + \omega - q)}{\sqrt{q^2 - \omega^2}} \int_{x=q}^{2\mu+\omega} dx \frac{(x^2 - q^2)^{3/2}}{x^2 - \omega^2}$$

$$= \frac{g}{16\pi} \frac{\Theta(q - \omega) \Theta(2\mu + \omega - q)}{\sqrt{q^2 - \omega^2}} \left[ x\sqrt{x^2 - q^2} - \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \ln|x + \sqrt{x^2 - q^2}| - \frac{2(\omega^2 - q^2)^{3/2}}{\omega} \arcsin \left( \frac{x}{q} \sqrt{\frac{q^2 - \omega^2}{x^2 - \omega^2}} \right) \right]_{x=q}^{2\mu+\omega}$$

$$= \frac{g}{16\pi} \frac{\Theta(q - \omega) \Theta(2\mu + \omega - q)}{\sqrt{q^2 - \omega^2}} \left[ (2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{q^2 - \omega^2}} - \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \ln\left( \frac{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}}{q} \right) - \frac{2(\omega^2 - q^2)^{3/2}}{\omega} \arcsin \left( \frac{2\mu + \omega}{q} \sqrt{\frac{q^2 - \omega^2}{(2\mu + \omega)^2 - \omega^2}} \right) \right].$$  \hspace{1cm} (6.25)

Similar calculations yield explicit expressions for the other terms involving cone-cone scattering,

$$I_2 = \frac{g}{16\pi} \frac{\Theta(q - \omega) \Theta(2\mu - \omega - q)}{\sqrt{q^2 - \omega^2}} \left[ -(2\mu - \omega) \sqrt{\frac{(2\mu - \omega)^2 - q^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \ln\left( \frac{2\mu - \omega + \sqrt{(2\mu - \omega)^2 - q^2}}{q} \right) \right.$$

$$+ \frac{2\omega^2 - q^2}{\omega} \arcsin \left( \frac{2\mu - \omega}{q} \sqrt{\frac{q^2 - \omega^2}{(2\mu - \omega)^2 - \omega^2}} \right) \right].$$  \hspace{1cm} (6.26)
\[ I_3 = \frac{g}{16\pi} \Theta(\omega - q) \Theta(q - |2\mu - \omega|) \]
\[ \times \left[ -(2\mu - \omega) \sqrt{\frac{q^2 - (2\mu - \omega)^2}{\omega^2 - q^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} \arccos \left( \frac{2\mu - \omega}{q} \right) 
+ 2\frac{\omega^2 - q^2}{\omega} \arccos \left( \frac{2\mu - \omega}{q} \sqrt{\frac{\omega^2 - q^2}{\omega^2 - (2\mu - \omega)^2}} \right) \right] \] (6.27)
\[ + \frac{g}{16\pi} \Theta(\omega - q - 2\mu) \left[ \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2} - 2\omega} \pi + 2\frac{\omega^2 - q^2}{\omega} \pi \right]. \]

The final contribution to the imaginary part, \( I_4 \), involves scattering from the flat band. This lends a simple delta function, \( \delta(\omega - k) \), which allows for the immediate evaluation of the integral over \( dk \),
\[ I_4 = \frac{g}{4\pi} \Theta(\omega - \mu) \omega \int_{-\pi}^{\pi} d\theta \frac{q^2 \sin^2 \theta}{2(\omega^2 + q^2 + 2q\omega \cos \theta)} \] (6.28)

What remains is a standard angular integral whose identity is derived in the Appendix and given in Eq. (A.13),
\[ I_4 = \frac{g}{16\pi} \Theta(\omega - \mu) q \int_{-\pi}^{\pi} d\theta \frac{\sin^2 \theta}{(\omega^2 + q^2)/2q\omega + \cos \theta} \]
\[ = \frac{g}{16\pi} \Theta(\omega - \mu) q \left[ 2\pi \left( \frac{\omega^2 + q^2}{2q\omega} - \sqrt{\left( \frac{\omega^2 + q^2}{2q\omega} \right)^2 - 1} \right) \right] \] (6.29)
\[ = \frac{g}{16\pi} \Theta(\omega - \mu) \left[ \frac{\omega^2 + q^2 - |\omega^2 - q^2|}{\omega} \pi \right] \]
\[ = \frac{g}{16\pi} \Theta(\omega - \mu) \left[ \frac{2 \min(\omega^2, q^2)}{\omega} \pi \right]. \]

The summation of Eqs. (6.25)-(6.27) and (6.29) gives the total imaginary part of the
dice polarizability,

\[
\text{Im } Q = I_1 + I_2 + I_3 + I_4 \\
= \frac{g}{16\pi} \Theta(q - \omega) \Theta(2\mu + \omega - q) \\
\times \left[ (2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \ln \left| \frac{q}{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}} \right| \\
- \frac{2\omega^2 - q^2}{\omega} \arccos \left( \frac{2\mu + \omega}{2q} \sqrt{\frac{q^2 - \omega^2}{\mu(\omega + \mu)}} \right) \right] \\
+ \frac{g}{16\pi} \Theta(q - \omega) \Theta(2\mu - \omega - q) \\
\times \left[ -(2\mu - \omega) \sqrt{\frac{(2\mu - \omega)^2 - q^2}{q^2 - \omega^2}} - \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \ln \left| \frac{q}{2\mu - \omega + \sqrt{(2\mu - \omega)^2 - q^2}} \right| \\
+ \frac{2\omega^2 - q^2}{\omega} \arccos \left( \frac{2\mu - \omega}{2q} \sqrt{\frac{q^2 - \omega^2}{\mu(\omega - \mu)}} \right) \right] \\
+ \frac{g}{16\pi} \Theta(q - \omega - 2\mu) \left[ \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} \pi + \frac{2\omega^2 - q^2}{\omega} \pi \right] \\
+ \frac{g}{16\pi} \Theta(\omega - \mu) \left[ 2\min(\omega^2, q^2) \pi \right].
\]

Equation (6.30) is plotted over the whole \((q, \omega)\) space in Fig. 6.3 with cuts provided in Figs. 6.4 and 6.5. These latter two figures make the flat-band scattering contributions explicit by colouring them orange. \(\text{Im } Q\) in the dice lattice shows many similarities and some important differences when compared to graphene.

The presence of the flat band has two broad impacts on the dice polarizability in its comparison to graphene. The first is direct, where we include scattering from the flat band \((I_4)\). The other impact is an indirect one, where the presence of the flat band extends the Hilbert space in the \(s = 1\) system (with its 3-spinor wavefunction) relative to the \(s = 1/2\)
system (2-spinor). This extension leads to a richer behaviour in the cone-cone scattering, Eq. (6.9). That is, the mere presence of the flat band affects scattering events in which it is not directly involved.

Several manipulations can be made on the expression in Eq. (6.30) that remove the effects of the flat band and lead to the graphene expression in Eq. (6.1). The first step in this transformation is the omission of $I_4$ (Eq. (6.29)) from the result, the term that is a result of scattering from the flat band. This is the last line in the full solution, Eq. (6.30).

To account for the indirect effects of the flat band, the piece in square brackets in the second-to-last line of Eq. (6.30) is replaced by $\pi q^2/\omega$. Next, the factor $3q^2 - 2\omega^2$ as it appears elsewhere in the lines above is replaced by $q^2$. Finally, the arccos terms proportional to $(\omega^2 - q^2)/\omega$ are omitted entirely.

These latter considerations due to the extended Hilbert space lead to minor differences in the cone-cone scattering when comparing the graphene and dice systems. It is the scattering from the flat band, $I_4$, that significantly impacts the polarizability. Seen in Fig. 6.3, there is a discontinuous step up in $\text{Im } Q$ at $\omega = \mu$ as result of this term. The PHC relative to
Figure 6.4: Imaginary part of the dice polarizability function along $q$ for four different values of $\omega$. The cuts in panels (b) and (c) are respectively situated just below and above the step at $\omega = \mu$. In panels (c) and (d), the non-zero contribution from flat band scattering is coloured orange.
Figure 6.5: Imaginary part of the dice polarizability function along $\omega$ for four different values of $q$. Contributions from flat-band scattering are coloured orange.
Figure 6.6: Particle-hole continuum in the dice lattice. Contributions from cone-cone scattering are shaded grey, intra-cone marked with a grid and inter-cone with dots. The flat-cone contribution is overlaid with red transparency.

graphene is greatly extended by this step.

Figure 6.6 outlines the PHC in the dice lattice indicating its different contributions. Like graphene, there is a contribution due to inter-cone scattering bound by $\omega < q < 2\mu + \omega$ (grey dots), as well as the intra-cone piece (grey grid) in much of the $q < \omega$ region. Overlaid on top of the graphene PHC is the contribution due to scattering from the flat band (red transparency), present for all $\omega > \mu$. This extension of the PHC reflects the fact that for any value of momentum, it is possible to scatter a flat-band state into the upper cone, provided the energy is large enough to overtake the Fermi level at $\omega = \mu$ (see the $s = 1$ dispersion in Fig. 3.1). The discontinuous step up in $\text{Im} Q$ leads to a logarithmic divergence along the same line, $\omega = \mu$, in the Kramers-Kronig related real part. This in turn leads to a large screening effect arising from the singular density of states found in the flat band.
Real Part

From Eq. (6.3), the real part of the dice polarizability is

\[
\text{Re} Q(q, \omega) = \frac{g}{4\pi^2} \int d^2k \sum_{\lambda, \lambda'} P^{n_f}(\varepsilon'_{\lambda}(k')) - n_f(\varepsilon_{\lambda}(k)) \frac{F_{\lambda\lambda'}(k)}{\omega - (\varepsilon'_{\lambda}(k') - \varepsilon_{\lambda}(k))}.
\]

(6.31)

There are six non-zero terms from the summation over \( \lambda \) and \( \lambda' \),

\[
J_1 = \frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{++}(k)}{\omega + k}, \quad J_2 = -\frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{++}(k)}{\omega - k'},
\]

\[
\tilde{J}_3 = \frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{+-}(k)}{\omega + k + k'}, \quad \tilde{J}_4 = -\frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{+-}(k)}{\omega - k - k'},
\]

\[
\tilde{J}_5 = -\frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{++}(k)}{\omega + k - k'}, \quad \tilde{J}_6 = \frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(k - \mu) \frac{F_{++}(k)}{\omega - k + k'}.
\]

(6.32)

The four terms \( \tilde{J}_3, \tilde{J}_4, \tilde{J}_5, \) and \( \tilde{J}_6 \) are difficult to solve and so they are rearranged into more tractable forms. In the first two, the step function is split up into a \( \mu \to 0 \) piece with a finite-\( \mu \) correction, \( \Theta(k - \mu) = 1 - \Theta(\mu - k) \). The finite-\( \mu \) corrections in \( \tilde{J}_3 \) and \( \tilde{J}_4 \) are added to \( \tilde{J}_5 \) and \( \tilde{J}_6 \), respectively (the terms in each pairing share the same sign), giving

\[
J_3 = -\frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(\mu - k) \left( \frac{F_{++}(k)}{\omega + k - k'} + \frac{F_{+-}(k)}{\omega + k + k'} \right),
\]

\[
J_4 = \frac{g}{4\pi^2} \int d^2k \mathcal{P} \Theta(\mu - k) \left( \frac{F_{++}(k)}{\omega + k + k'} + \frac{F_{+-}(k)}{\omega - k - k'} \right).
\]

(6.33)

The remaining pieces (those unrestricted in \( k \)) are combined and will require a Kramers-Kronig transformation of the imaginary part in order to solve,

\[
J_5 = \frac{g}{4\pi^2} \int d^2k \mathcal{P} F_{+-}(k) \left( \frac{1}{\omega + k + k'} - \frac{1}{\omega - k - k'} \right).
\]

(6.34)

After this rearrangement, the full real part of the polarizability is the sum of five terms,

\[
\text{Re} Q(q, \omega) = \sum_{j=1}^{5} J_j.
\]

(6.35)
From this point forward, the notation $P$ is dropped for brevity. It is understood that each of the $J_i$ involves integration over the principal part (Eq. (2.22)).

The first of the integrals to be solved, $J_1$, involves scattering from the flat band. With one band fixed at zero energy, this integral (and its companion $J_2$) is simpler to solve than the cone-cone terms, $J_3$ and $J_4$. In terms of the integration variables $k = (k, \theta)$, the scattering amplitude involving the flat band is, from Eq. (6.8),

$$F_{z0}(k) = \sin^2 \varphi_k$$

$$= 1 - \cos^2 \varphi_k$$

$$= \frac{q^2 \sin^2 \theta}{k^2 + q^2 + 2qk\cos \theta}. \tag{6.36}$$

In solving $J_1$, the standard integral in Eq. (A.13) is used to trace out $d\theta$,

$$J_1 = \frac{g}{4\pi^2} \int_{-\infty}^{\infty} \frac{dk}{k + \omega} \int_{-\pi}^{\pi} d\theta F_{z0}(k)$$

$$= \frac{g}{16\pi^2 q} \int_{-\infty}^{\infty} \frac{dk}{k + \omega} \int_{-\pi}^{\pi} d\theta \frac{\sin^2 \theta}{(k^2 + q^2)^2/2qk + \cos \theta}$$

$$= \frac{g}{8\pi q} \int_{-\infty}^{\infty} \frac{dk}{k + \omega} \left( \frac{k^2 + q^2}{2qk} - \sqrt{\frac{k^2 + q^2}{2qk}} - 1 \right)$$

$$= \frac{g}{8\pi q} \int_{-\infty}^{\infty} \frac{dk}{k + \omega} \left( \Theta(q - k)k^2 + \Theta(k - q)q^2 \right)$$

$$= \frac{g}{8\pi} \left[ \Theta(q - \mu) \int_{\mu}^{q} dk \frac{k}{k + \omega} + \Theta(q - \mu) \int_{q}^{\infty} dk \frac{k^2}{k(k + \omega)} + \Theta(\mu - q) \int_{\mu}^{q} dk \frac{q^2}{k(k + \omega)} \right]$$

$$+ \frac{g}{16\pi} \Theta(q - \mu) \left[ 2q - 2\mu + 2\omega \ln \left( \frac{\omega + \mu}{\omega + q} \right) + 2q^2 \omega \ln \left( \frac{\omega + q}{q} \right) \right]$$

$$+ \frac{g}{16\pi} \Theta(\mu - q) \left[ 2q^2 \omega \ln \left( \frac{\omega + \mu}{\mu} \right) \right]. \tag{6.37}$$

The solution to $J_2$, being the other flat-band term, follows from a similar procedure as $J_1$,
yielding

\[
J_2 = \frac{g}{16\pi} \Theta(q - \mu) \left[ 2q - 2\mu + 2\omega \ell n \left| \frac{\omega - q}{\omega - \mu} \right| + 2\frac{q^2}{\omega} \ell n \left| \frac{q}{\omega - q} \right| \right] \\
+ \frac{g}{16\pi} \Theta(\mu - q) \left[ 2\frac{q^2}{\omega} \ell n \left| \frac{\mu}{\omega - \mu} \right| \right].
\] (6.38)

Solutions to the cone-cone scattering terms are much more involved. The first is

\[
J_3 = -\frac{g}{4\pi^2} \int_0^\mu dk \int_{-\pi}^\pi d\theta \left( \frac{F_{++}(k)}{\omega + k - k'} + \frac{F_{+-}(k)}{\omega + k + k'} \right).
\] (6.39)

In the round brackets,

\[
\frac{F_{++}(k)}{\omega + k - k'} + \frac{F_{+-}(k)}{\omega + k + k'} = \frac{(k + q \cos \theta + k')^2(\omega + k + k') + (k + q \cos \theta - k')^2(\omega + k - k')}{4(k')^2[(\omega + k)^2 - (k')^2]}
\]

\[
= \frac{2(\omega + k)((k + q \cos \theta)^2 + (k')^2 + 4(k')^2(k + q \cos \theta)}{4(k')^2(2\omega k + \omega^2 - q^2 - 2q k \cos \theta)}
\]

\[
= \frac{3k + \omega + 2q \cos \theta}{2(2\omega k + \omega^2 - q^2 - 2q k \cos \theta)}
\]

\[
+ \frac{2((k^2 + q^2)(2\omega k + \omega^2 - q^2) + 2q k(\omega^2 - 2q^2 + 2\omega k - k^2)) \cos \theta - 4q^2 k^2 \cos^2 \theta}{4q k \cos \theta - a_1 - \frac{1}{2k \cos \theta - a_1} - \frac{1}{8q^2 \cos^2 \theta + a_2 \cos \theta + b_2} - \frac{1}{8q^2 \cos^2 \theta + a_2 \cos \theta + b_2}}
\]

\[
- \frac{\omega + k}{\omega + k} - \frac{\omega + k}{\omega + k} - \frac{\omega + k}{\omega + k} - \frac{\omega + k}{\omega + k}.
\] (6.40)

where

\[
a_1 = \frac{1}{2q k}(2\omega k + \omega^2 - q^2),
\]

\[
a_2 = \frac{1}{2q k}(k^2 - 2\omega k + 2q^2 - \omega^2),
\] (6.41)

\[
b_2 = -\frac{1}{4q^2 k^2}(k^2 + q^2)(2\omega k + \omega^2 - q^2).
\]

Then

\[
J_3 = \frac{g}{8\pi^2} \int_0^\mu dk \left[ \frac{3k + \omega}{2q} A_1 + A_2 + \frac{k(\omega + k)}{4q^2} A_3 + \frac{\omega + k}{2q} A_4 + \frac{\omega + k}{4k} A_5 \right],
\] (6.42)
which involves standard integrals solved in the Appendix,

\[ A_1 = \int_{-\pi}^{\pi} d\theta \frac{1}{\cos \theta - a_1}, \quad A_2 = \int_{-\pi}^{\pi} d\theta \frac{\cos \theta}{\cos \theta - a_1}, \quad A_3 = \int_{-\pi}^{\pi} d\theta \frac{1}{\cos^2 \theta + a_2 \cos \theta + b_2}, \]
\[ A_4 = \int_{-\pi}^{\pi} d\theta \frac{\cos \theta}{\cos^2 \theta + a_2 \cos \theta + b_2}, \quad A_5 = \int_{-\pi}^{\pi} d\theta \frac{\cos \theta}{\cos^2 \theta + a_2 \cos \theta + b_2}. \]  
\[ (6.43) \]

The solutions to the first two of the \( d\theta \) integrals are given in Eqs. (A.3) and (A.4), respectively. Writing \( a_1 \to a \) for brevity,

\[ A_1 = \frac{-2\pi}{\sqrt{a^2 - 1}} \text{sgn}(a) \Theta(a^2 - 1), \quad A_2 = 2\pi - 2\pi \frac{a}{\sqrt{a^2 - 1}} \text{sgn}(a) \Theta(a^2 - 1). \]  
\[ (6.44) \]

These are non-zero only for \( a^2 > 1 \), implying

\[ 4\omega^2 k^2 + 4\omega(\omega^2 - q^2)k + (\omega^2 - q^2)^2 > 4q^2 k^2 \]
\[ (\omega^2 - q^2)[(2k + \omega)^2 - q^2] > 0. \]  
\[ (6.45) \]

Two cases arise,

1. \( \omega > q \). The inequality above would then imply that \( 2k + \omega > q \), which is already covered by the condition \( \omega > q \). In addition, \( a \) is positive in this case.

2. \( \omega < q \). Here, the inequality implies \( 2k + \omega < q \), which covers the condition \( \omega < q \). In this case, \( a \) is negative.

With these considerations,

\[ \text{sgn}(a) \Theta(a^2 - 1) = \Theta(\omega - q) - \Theta(q - \omega - 2k). \]  
\[ (6.46) \]

Also,

\[ \frac{1}{\sqrt{a^2 - 1}} = \frac{2qk}{\sqrt{(\omega^2 - q^2)[(2k + \omega)^2 - q^2]}}, \quad \frac{a}{\sqrt{a^2 - 1}} = \frac{2\omega k + \omega^2 - q^2}{\sqrt{(\omega^2 - q^2)[(2k + \omega)^2 - q^2]}}. \]  
\[ (6.47) \]
Thus,

\[
A_1 = 2\pi \frac{2qk}{\sqrt{(\omega^2 - q^2)(2k + \omega)^2 - q^2}} \left[ \Theta(\omega - 2k) - \Theta(\omega - q) \right],
\]

\[
A_2 = 2\pi + 2\pi \frac{2\omega k + \omega^2 - q^2}{\sqrt{(\omega^2 - q^2)(2k + \omega)^2 - q^2}} \left[ \Theta(\omega - 2k) - \Theta(\omega - q) \right].
\]

For the three remaining integrals (whose solutions are given in Eqs. (A.8), (A.10), and (A.12), respectively), we now take \(a_2 \to a\) and \(b_2 \to b\),

\[
A_3 = 8\pi \left( \frac{\zeta_1 \Theta(1 - |\zeta_1|)}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \text{perm.} \right),
\]

\[
A_4 = 4\pi \left( \frac{(\zeta_1^2 + q) \Theta(1 - |\zeta_1|)}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \text{perm.} \right),
\]

\[
A_5 = 2\pi + 2\pi \left( \frac{(\zeta_1^2 + 1)^2 \Theta(1 - |\zeta_1|)}{\zeta_1(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \text{perm.} \right),
\]

where ‘perm.’ indicates permutations of the first term over the four parameters

\[
\zeta_1 = \frac{1}{2} \left( -a - \sqrt{a^2 - 4b} - \sqrt{2(a^2 - 2b - 2 + a\sqrt{a^2 - 4b})} \right),
\]

\[
\zeta_2 = \frac{1}{2} \left( -a - \sqrt{a^2 - 4b} + \sqrt{2(a^2 - 2b - 2 + a\sqrt{a^2 - 4b})} \right),
\]

\[
\zeta_3 = \frac{1}{2} \left( -a + \sqrt{a^2 - 4b} - \sqrt{2(a^2 - 2b - 2 - a\sqrt{a^2 - 4b})} \right),
\]

\[
\zeta_4 = \frac{1}{2} \left( -a + \sqrt{a^2 - 4b} + \sqrt{2(a^2 - 2b - 2 - a\sqrt{a^2 - 4b})} \right).
\]

In terms of \(q\) and \(k\),

\[
\zeta_1 = \frac{1}{2qk} (-k^2 - q^2 - |k^2 - q^2|) = -\frac{\max(k^2, q^2)}{qk},
\]

\[
\zeta_2 = \frac{1}{2qk} (-k^2 - q^2 + |k^2 - q^2|) = -\frac{\min(k^2, q^2)}{qk}.
\]

Since the solutions to \(A_3\), \(A_4\), and \(A_5\) are symmetric under \(\zeta_1 \leftrightarrow \zeta_2\), we are free to choose

\[
\zeta_1 = -\frac{q}{k}, \quad \zeta_2 = -\frac{k}{q}.
\]
In addition,
\[
\zeta_3 = \frac{1}{2qk} \left( 2\omega k + \omega^2 - q^2 - \sqrt{(\omega^2 - q^2)((2k + \omega)^2 - q^2)} \right),
\]
\[
\zeta_4 = \frac{1}{2qk} \left( 2\omega k + \omega^2 - q^2 + \sqrt{(\omega^2 - q^2)((2k + \omega)^2 - q^2)} \right).
\]

(6.53)

As for the step functions, the first two are simple:
\[
\Theta(1 - |\zeta_1|) = \Theta(k - q), \quad \Theta(1 - |\zeta_2|) = \Theta(q - k).
\]

(6.54)

The magnitudes of $|\zeta_3|$ and $|\zeta_4|$, on the other hand, depend on whether the quantity
\[
s = \sqrt{(\omega^2 - q^2)((2k + \omega)^2 - q^2)}
\]

(6.55)
is real or imaginary. In the case of $s \in \mathbb{I}$, there is no contribution to any of $A_3$, $A_4$, or $A_5$. What happens in that case is that during contour integration (after making a change of variables to $z = e^{i\theta}$), the $\zeta_i$’s represent poles in the integrand. If $s \in \mathbb{I}$, then $\zeta_3$ and $\zeta_4$ both lie on the unit circle contour, $|z| = 1$. Because these are integrals over the principal part, poles lying on the contour are ignored. Thus, for non-zero contributions, it must be that $s \in \mathbb{R}$, or
\[
(\omega^2 - q^2)[(2k + \omega)^2 - q^2] > 0.
\]

(6.56)

Two cases arise that satisfy this inequality,

1. Case 1: $\omega > q$ and $2k + \omega > q$. Multiplying these two conditions gives $2\omega k + \omega^2 > q^2$.

2. Case 2: $\omega < q$ and $2k + \omega < q$. Multiplication gives $2\omega k + \omega^2 < q^2$.

Suppose that $|\zeta_3|^2 < 1$. Then
\[
(2\omega k + \omega^2 - q^2)\sqrt{(\omega^2 - q^2)((2k + \omega)^2 - q^2)} > (\omega^2 - q^2)[(2k + \omega)^2 - q^2]
\]
\[
2\omega k + \omega^2 - q^2 > \sqrt{(\omega^2 - q^2)((2k + \omega)^2 - q^2)} > 0.
\]

(6.57)

This falls within case 1 above. If, instead, $|\zeta_4|^2 < 1$, then $2\omega k + \omega^2 - q^2 < 0$, falling into
case 2. This all leads to

$$\Theta(1 - |\zeta_3|) = \Theta(\omega - q) , \ \Theta(1 - |\zeta_4|) = \Theta(q - \omega - 2k). \quad (6.58)$$

Extensive algebra gives

$$\begin{align*}
\zeta_1 &= \frac{-q^2 k^2}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} , \\
\zeta_2 &= \frac{q^2 k^2}{(\zeta_2 - \zeta_1)(\zeta_2 - \zeta_3)(\zeta_2 - \zeta_4)} , \\
\zeta_3 &= \frac{-q^2 k^2}{(\zeta_3 - \zeta_1)(\zeta_3 - \zeta_2)(\zeta_3 - \zeta_4)} , \\
\zeta_4 &= \frac{q^2 k^2}{(\zeta_4 - \zeta_1)(\zeta_4 - \zeta_2)(\zeta_4 - \zeta_3)} .
\end{align*} \quad (6.59)$$

Thus,

$$A_3 = 8\pi \frac{q^2 k^2}{(\omega + k)^2} \left( \Theta(1 - |\zeta_2|) - \Theta(1 - |\zeta_1|) \frac{k^2 - q^2}{\sqrt{(\omega^2 - q^2)(\omega^2 - q^2)}} + \Theta(1 - |\zeta_4|) - \Theta(1 - |\zeta_3|) \frac{-q^2 k^2}{\sqrt{(\omega^2 - q^2)(\omega^2 - q^2)}} \right) ,$$

$$\quad = 8\pi \frac{q^2 k^2}{(\omega + k)^2} \left( -\frac{\text{sgn} (k-q)}{k^2 - q^2} + \Theta(q - \omega - 2k) - \Theta(q - \omega) \right) . \quad (6.60)$$

Similarly,

$$A_4 = 4\pi \frac{qk}{(\omega + k)^2} \left\{ \frac{k^2 + q^2}{k^2 - q^2} \text{sgn} (k-q) + \frac{2\omega k + \omega^2 - q^2}{\sqrt{(\omega^2 - q^2)(2k + \omega)^2 - q^2}} [\Theta(q - \omega - 2k) - \Theta(\omega - q)] \right\} , \quad (6.61)$$

$$A_5 = 2\pi + \frac{2\pi}{(\omega + k)^2} \left\{ -\frac{(k^2 + q^2)^2}{k^2 - q^2} \text{sgn} (k-q) \\
\quad + \frac{(2\omega k + \omega^2 - q^2)^2}{\sqrt{(\omega^2 - q^2)(2k + \omega)^2 - q^2}} [\Theta(q - \omega - 2k) - \Theta(\omega - q)] \right\} . \quad (6.62)$$
Subbing these solutions into Eq. (6.42) and rearranging gives

\[
J_3 = \frac{g}{16\pi} \int_0^\mu dk \left( 4 + \frac{\omega + k}{k} - \frac{k^2 - q^2}{k(\omega + k)} \text{sgn}(k - q) \right.
\]

\[
- 4 \sqrt{\frac{(2k + \omega)^2 - q^2}{\omega^2 - q^2}} \left[ \Theta(q - \omega - 2k) + \Theta(\omega - q) \right]
\]

\[
+ \sqrt{\frac{(\omega^2 - q^2)(2k + \omega)^2 - q^2}{k(\omega + k)}} \left[ \Theta(q - \omega - 2k) - \Theta(\omega - q) \right] \right).
\]

(6.63)

The five major terms in Eq. (6.63) are labelled \( t_1, ... t_5 \) and solved in turn. The first is straightforward,

\[
t_1 = \frac{g}{16\pi} \int_0^\mu dk 4 = \frac{g}{16\pi} 4\mu.
\]

(6.64)

The next term involves a divergent piece,

\[
t_2 = \frac{g}{16\pi} \int_0^\mu dk \frac{(\omega + k)}{k}
\]

\[
= \frac{g}{16\pi} \mu + \frac{g}{16\pi} \omega \ell n \left| \frac{\mu}{\epsilon} \right| \text{, where } \epsilon \rightarrow 0^+ \text{ is a low-} k \text{ cutoff}
\]

(6.65)

Proceeding forward,

\[
t_3 = -\frac{g}{16\pi} \int_0^\mu dk \frac{k^2 - q^2}{k(\omega + k)} \text{sgn}(k - q)
\]

\[
= \frac{g}{16\pi} \left[ \int_0^{\min(q, \mu)} dk - \Theta(\mu - q) \int_q^\mu dk \right] \frac{k^2 - q^2}{k(\omega + k)}
\]

\[
= \frac{g}{16\pi} \left[ k \frac{-q^2}{\omega} \ell n |k| - \frac{\omega^2 - q^2}{\omega} \ell n |\omega + k| \right]
\]

\[
\left\{ \begin{array}{l}
\int_{k=0}^{\min(q, \mu)} dk - \Theta(\mu - q) \int_{k=q}^\mu dk \\end{array} \right\}
\]

\[
= \frac{g}{16\pi} \Theta(\mu - q) \left[ 2q - \mu - \frac{q^2}{\omega} \ell n \left| \frac{\mu}{\epsilon} \right| + \frac{q^2}{\omega} \ell n \left| \frac{\mu}{q} \right| - \frac{\omega^2 - q^2}{\omega} \ell n \left| \frac{(\omega + q)^2}{\omega(\omega + \mu)} \right| \right]
\]

\[
\left. + \frac{g}{16\pi} \Theta(q - \mu) \left[ \mu - \frac{q^2}{\omega} \ell n \left| \frac{\mu}{\epsilon} \right| - \frac{\omega^2 - q^2}{\omega} \ell n \left| \frac{\omega + \mu}{\omega} \right| \right] \right)
\]

(6.66)

\[
= \frac{g}{16\pi} \Theta(\mu - q) \left[ 2q - \mu + \frac{2q^2}{\omega} \ell n \left| \frac{\mu}{q} \right| + \frac{\omega^2 - q^2}{\omega} \ell n \left| \frac{\omega(\omega + \mu)}{(\omega + q)^2} \right| \right]
\]

\[
+ \frac{g}{16\pi} \Theta(q - \mu) \left[ \mu + \frac{\omega^2 - q^2}{\omega} \ell n \left| \frac{\omega}{\omega + \mu} \right| \right]
\]

\[
+ \frac{g}{16\pi} \left[ -q^2 \ell n \left| \frac{\mu}{\epsilon} \right| \right].
\]
Next,

\[ t_4 = -\frac{g}{16\pi} \int_{0}^{\mu} dk \, 4 \sqrt{(2k + \omega)^2 - q^2} \left[ \Theta(q - \omega - 2\mu) + \Theta(\omega - q) \right] \]

\[ = -\frac{g}{16\pi} \frac{4\Theta(q - \omega)}{\sqrt{q^2 - \omega^2}} \int_{0}^{\min(\mu, \frac{q - \omega}{2})} dk \, \sqrt{q^2 - (2k + \omega)^2} \]

\[ - \frac{g}{16\pi} \frac{4\Theta(\omega - q)}{\sqrt{\omega^2 - q^2}} \int_{0}^{\mu} dk \, \sqrt{(2k + \omega) - q^2} \]

\[ = -\frac{g}{16\pi} \frac{2\Theta(q - \omega)}{\sqrt{q^2 - \omega^2}} \int_{0}^{\min(2\mu + \omega, q)} dx \, \sqrt{q^2 - x^2} - \frac{g}{16\pi} \frac{2\Theta(\omega - q)}{\sqrt{\omega^2 - q^2}} \int_{0}^{\mu} dx \, \sqrt{x^2 - q^2} \]

\[ = -\frac{g}{16\pi} \frac{\Theta(q - \omega)}{\sqrt{q^2 - \omega^2}} \left[ x\sqrt{q^2 - x^2} + q^2 \arcsin \left( \frac{x}{q} \right) \right]_{x=\omega}^{\min(2\mu + \omega, q)} - \frac{g}{16\pi} \frac{\Theta(\omega - q)}{\sqrt{\omega^2 - q^2}} \left[ x\sqrt{x^2 - q^2} - q^2 \ln \left( x + \sqrt{x^2 - q^2} \right) \right]_{x=\omega}^{2\mu + \omega} \]

\[ = \frac{g}{16\pi} \Theta(q - \omega - 2\mu) \left[ - (2\mu + \omega) \sqrt{\frac{q^2 - (2\mu + \omega)^2}{q^2 - \omega^2}} + \frac{q^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu + \omega}{q} \right) \right] \]

\[ + \frac{g}{16\pi} \Theta(q - \omega) \left[ \omega - \frac{q^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{\omega}{q} \right) \right] \]

\[ + \frac{g}{16\pi} \Theta(\omega - q) \left[ \omega - (2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{q^2}{\sqrt{\omega^2 - q^2}} \left( \frac{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}}{\omega + \sqrt{\omega^2 - q^2}} \right) \right]. \]

(6.67)
Finally,

\[
t_5 = \frac{g}{16\pi} \int_0^\mu dk \frac{\sqrt{\omega^2 - q^2}[(2k + \omega)^2 - q^2]}{k(\omega + k)} [\Theta(q - \omega - 2k) - \Theta(\omega - q)]
\]

\[
= \frac{g}{16\pi} \Theta(q - \omega) \sqrt{q^2 - \omega^2} \int_0^{\min(\mu, \frac{q}{\omega})} dk \frac{\sqrt{q^2 - (2k + \omega)^2}}{k(\omega + k)}
\]

\[
- \frac{g}{16\pi} \Theta(\omega - q) \sqrt{\omega^2 - q^2} \int_0^\mu dk \frac{\sqrt{(2k + \omega)^2 - q^2}}{k(\omega + k)}
\]

\[
= \frac{g}{16\pi} \Theta(q - \omega) \sqrt{q^2 - \omega^2} \int_\omega^{\min(2\mu + \omega, q)} dx \frac{2\sqrt{q^2 - x^2}}{x^2 - \omega^2}
\]

\[
- \frac{g}{16\pi} \Theta(\omega - q) \sqrt{\omega^2 - q^2} \int_\omega^{2\mu + \omega} dx \frac{2\sqrt{x^2 - q^2}}{x^2 - \omega^2}
\]

\[
= \frac{g}{16\pi} \Theta(q - \omega - 2\mu) \left[ 2\sqrt{q^2 - \omega^2} \arccos \left( \frac{2\mu + \omega}{q} \right) \right.
\]

\[
+ \frac{\omega^2 - q^2}{\omega} \left| \ln \frac{\omega \sqrt{q^2 - (2\mu + \omega)^2} + (2\mu + \omega) \sqrt{\omega^2 - q^2}}{\omega \sqrt{q^2 - (2\mu + \omega)^2} - (2\mu + \omega) \sqrt{\omega^2 - q^2}} \right|_{x=\omega}
\]

\[
+ \frac{g}{16\pi} \Theta(q - \omega) \left[ -2\sqrt{q^2 - \omega^2} \arccos \left( \frac{\omega}{q} \right) \right]
\]

\[
+ \frac{g}{16\pi} \Theta(\omega - q) \left[ -2\sqrt{\omega^2 - q^2} \ln \frac{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}}{\omega + \sqrt{\omega^2 - q^2}} \right.
\]

\[
+ \frac{\omega^2 - q^2}{\omega} \left| \ln \frac{\omega \sqrt{(2\mu + \omega)^2 - q^2} + (2\mu + \omega) \sqrt{\omega^2 - q^2}}{\omega \sqrt{(2\mu + \omega)^2 - q^2} - (2\mu + \omega) \sqrt{\omega^2 - q^2}} \right|_{x=\omega}
\]

\[
+ \frac{g}{16\pi} \left[ \frac{\omega^2 - q^2}{\omega} \ln \frac{2\omega(\omega^2 - q^2)}{q^2\omega} \right. - \frac{\omega^2 - q^2}{\omega} \ln \left. \frac{\mu}{\epsilon} \right|_{x=\omega} \right].
\]

(6.68)
Note that the last step in calculating $t_5$ involves the following evaluation (for $\omega > q$),

$$\ell_n \left| \frac{\omega \sqrt{x^2 - q^2} + x \sqrt{\omega^2 - q^2}}{\omega \sqrt{x^2 - q^2} - x \sqrt{\omega^2 - q^2}} \right|_{x = \omega^+} = \ell_n \left| \frac{2\omega \sqrt{\omega^2 - q^2}}{\omega \sqrt{(\omega + \epsilon)^2 - q^2} - (\omega + \epsilon) \sqrt{\omega^2 - q^2}} \right|$$

$$= \ell_n \left| \frac{2\omega (\omega^2 - q^2)}{q^2 \epsilon + \mathcal{O}(\epsilon^2)} \right|$$

$$= \ell_n \left| \frac{2\omega (\omega^2 - q^2)}{q^2 \mu} \right| + \ell_n \left| \frac{\mu}{\epsilon} \right| .$$

A similar evaluation in the $q > \omega$ case yields the same result.

Upon summation of the five terms, the divergent pieces involving $\epsilon$ cancel out exactly, yielding

$$J_3 = t_1 + t_2 + t_3 + t_4 + t_5$$

$$= \frac{g}{16\pi} \left[ 5\mu + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{q^2 \mu}{2\omega (\omega^2 - q^2)} \right| \right] + \frac{g}{16\pi} \Theta(q - \mu) \left[ 2q - \mu + \frac{2q^2}{\omega} \ell_n \left| \frac{\mu}{q} + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega (\omega + \mu)}{(\omega + q)^2} \right| \right] \right] + \frac{g}{16\pi} \Theta(\omega - q) \left[ \omega - (2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} \ell_n \left| \frac{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}}{\omega + \sqrt{\omega^2 - q^2}} \right| + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{(2\mu + \omega)^2 - q^2} + (2\mu + \omega) \sqrt{\omega^2 - q^2}}{\omega \sqrt{(2\mu + \omega)^2 - q^2} - (2\mu + \omega) \sqrt{\omega^2 - q^2}} \right| \right] + \frac{g}{16\pi} \Theta(q - \omega - 2\mu) \left[ -(2\mu + \omega) \sqrt{\frac{q^2 - (2\mu + \omega)^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu + \omega}{q} \right) \right] + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{q^2 - (2\mu + \omega)^2} + (2\mu + \omega) \sqrt{q^2 - \omega^2}}{\omega \sqrt{q^2 - (2\mu + \omega)^2} - (2\mu + \omega) \sqrt{q^2 - \omega^2}} \right| + \frac{g}{16\pi} \Theta(q - \omega) \left[ \omega + \frac{2\omega^2 - 3q^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{\omega}{q} \right) \right] .$$

(6.70)
Derived in a similar way to \( J_3 \), the other cone-cone term is

\[
J_4 = \frac{g}{16\pi} \left[ 5\mu + \frac{\omega^2 - q^2}{\omega} \ln \left( \frac{2\omega(\omega^2 - q^2)}{q^2\mu} \right) \right] + \frac{g}{16\pi} \Theta(q - \mu) \left[ \mu + \frac{\omega^2 - q^2}{\omega} \ln \left( \frac{\omega - \mu}{\omega} \right) \right] \\
+ \frac{g}{16\pi} \Theta(\mu - q) \left[ 2q - \mu + \frac{2q^2}{\omega} \ln \left( \frac{q}{\mu} \right) + \frac{\omega^2 - q^2}{\omega} \ln \left( \frac{(\omega - q)^2}{\omega(\omega - \mu)} \right) \right] \\
+ \frac{g}{16\pi} \Theta(q - \omega) \Theta(\omega + q - 2\mu) \\
\times \left[ -(2\mu - \omega) \sqrt{\frac{q^2 - (2\mu - \omega)^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu - \omega}{q} \right) \right] \\
+ \frac{g}{16\pi} \Theta(q - \omega) \left[ -\omega + \frac{2\mu^2 - 3q^2}{2\sqrt{q^2 - \omega^2}} \arccos \left( \frac{-\omega}{q} \right) \right] \\
+ \frac{g}{16\pi} \Theta(\omega - q) \Theta(2\mu - \omega - q) \\
\times \left[ |2\mu - \omega| \sqrt{\frac{(2\mu - \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{2\mu^2 - 3q^2}{\sqrt{\omega^2 - q^2}} \ln \left( \frac{|2\mu - \omega| + \sqrt{(2\mu - \omega)^2 - q^2}}{q} \right) \right] \\
\times \left[ -\omega^2 - q^2 \ln \left( \frac{\omega \sqrt{(2\mu - \omega)^2 - q^2} + |2\mu - \omega| \sqrt{\omega^2 - q^2}}{\omega \sqrt{(2\mu - \omega)^2 - q^2} - |2\mu - \omega| \sqrt{\omega^2 - q^2}} \right) \right] \\
+ \frac{g}{16\pi} \Theta(\omega - q) \left[ -\omega + \frac{3q^2 - 2\omega^2}{2\sqrt{\omega^2 - q^2}} \ln \left( \frac{\omega + \sqrt{\omega^2 - q^2}}{q} \right) \right].
\] (6.71)

The remaining integral (zero-\( \mu \) cone-cone contribution) is difficult to solve directly,

\[
J_5 = \frac{g}{4\pi^2} \int d^2k \ F_{+-}(k) \left( \frac{1}{\omega + k + k'} - \frac{1}{\omega - k - k'} \right).
\] (6.72)

Instead, it is most convenient to make use of the Kramers-Kronig (KK) relation in Eq. (2.26) (Table 2.1 is used for reference). The KK-conjugate to \( J_5 \), found in the imaginary part of the polarizability, is \( I_3 \mid_{\mu=0} \). From Eq. (6.27),

\[
I_3 \bigg|_{\mu=0} = \frac{g}{16} \Theta(\omega - q) \left( \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} + 2\frac{\omega^2 - q^2}{\omega} \right).
\] (6.73)
This is split up into four separate terms,

\[
s_1(\omega) = \frac{g}{16} \Theta(\omega - q) \frac{3q^2}{\sqrt{\omega^2 - q^2}} , \quad s_2(\omega) = -\frac{g}{8} \Theta(\omega - q) \frac{\omega^2}{\sqrt{\omega^2 - q^2}},
\]

\[
s_3(\omega) = \frac{g}{8} \Theta(\omega - q) \omega , \quad s_4(\omega) = -\frac{g}{8} \Theta(\omega - q) \frac{q^2}{\omega}.
\]

(6.74)

The KK-conjugate to each \(s_i\) is labelled \(r_i\). Beginning with \(r_1\),

\[
r_1(\omega) = \frac{2}{\pi} \int_0^\infty du \mathcal{P} \frac{us_1(u)}{u^2 - \omega^2}
\]

\[
= \frac{g}{8\pi} 3q^2 \int_q^\infty du \mathcal{P} \frac{u}{\sqrt{u^2 - q^2}} \frac{1}{(u^2 - \omega^2)}
\]

\[
= \frac{g}{8\pi} 3q^2 \left[ \Theta(\omega - q) \int_q^\infty du \frac{u}{\sqrt{u^2 - q^2}} \frac{1}{(u^2 - \omega^2)}
\]

\[
+ \Theta(\omega - q) \int_q^\infty du \mathcal{P} \frac{u}{\sqrt{u^2 - q^2}} \frac{1}{(u^2 - \omega^2)} \right] \quad (6.75)
\]

\[
= \frac{g}{16\pi} \Theta(\omega - q) \frac{3\pi q^2}{\sqrt{q^2 - \omega^2}}.
\]

Each of the next two terms, \(s_2\) and \(s_3\), blow up as \(\omega \to \infty\), but not their sum, \(s_2 + s_3\),

\[
r_2(\omega) + r_3(\omega) = \frac{2}{\pi} \int_0^\infty du \mathcal{P} \frac{u [s_2(\omega) + s_3(\omega)]}{u^2 - \omega^2}
\]

\[
= \frac{g}{4\pi} \int_q^\infty du \mathcal{P} \frac{u^2(\sqrt{u^2 - q^2} - u)}{\sqrt{u^2 - q^2} \sqrt{u^2 - \omega^2}}
\]

\[
= \frac{g}{4\pi} \left[ \Theta(\omega - q) \int_q^\infty du \frac{u^2(\sqrt{u^2 - q^2} - u)}{\sqrt{u^2 - q^2} (u^2 - \omega^2)}
\]

\[
+ \Theta(\omega - q) \int_q^\infty du \mathcal{P} \frac{u^2(\sqrt{u^2 - q^2} - u)}{\sqrt{u^2 - q^2} (u^2 - \omega^2)} \right] \quad (6.76)
\]

\[
= \frac{g}{16\pi} \left[ -4q + 2\omega \ln \frac{\omega + q}{\omega - q} - \Theta(\omega - q) \frac{2\pi \omega^2}{\sqrt{q^2 - \omega^2}} \right].
\]
The final piece is

\[
\begin{align*}
    r_4(\omega) &= \frac{2}{\omega} \int_0^\infty du P \frac{u s_4(u)}{u^2 - \omega^2} \\
    &= -\frac{g}{4\pi} q^2 \int_q^\infty du P \frac{1}{u^2 - \omega^2} \\
    &= -\frac{g}{4\pi} q^2 \left[ \Theta(q - \omega) \int_q^\infty \frac{1}{u^2 - \omega^2} + \Theta(\omega - q) \int_q^\infty \frac{1}{u^2 - \omega^2} \right] \\
    &= \frac{g}{16\pi} \left[ -\frac{2q^2}{\omega} \ln \left| \frac{\omega + q}{\omega - q} \right| \right].
\end{align*}
\]

(6.77)

The sum of \( r_1, ..., r_4 \) gives

\[
J_5 = \frac{g}{16\pi} \left[ 2\frac{\omega^2 - q^2}{\omega} \ln \left| \frac{\omega + q}{\omega - q} \right| - 4q + \Theta(q - \omega) \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \right].
\]

(6.78)
Finally, the sum total of $J_1, \ldots, J_5$ gives the real part of the dice lattice polarizability,

$$\text{Re} Q(q, \omega) = J_1 + J_2 + J_3 + J_4 + J_5$$

$$= \frac{g}{16\pi} \left[ 8\mu + \frac{\omega^2 + q^2}{\omega} \ell_n \left| \frac{\omega + \mu}{\omega - \mu} \right| \right]$$

$$+ \frac{g}{16\pi} \Theta(q - \omega) \Theta(\omega + q - 2\mu) \times \left[ -(2\mu - \omega) \sqrt{\frac{q^2 - (2\mu - \omega)^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu - \omega}{q} \right) \right.$$

$$\left. + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{q^2 - (2\mu - \omega)^2} + (2\mu - \omega) \sqrt{q^2 - \omega^2}}{\omega \sqrt{q^2 - (2\mu - \omega)^2} - (2\mu - \omega) \sqrt{q^2 - \omega^2}} \right| \right]$$

$$+ \frac{g}{16\pi} \Theta(q - \omega - 2\mu) \left[ -(2\mu + \omega) \sqrt{\frac{q^2 - (2\mu + \omega)^2}{q^2 - \omega^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{q^2 - \omega^2}} \arccos \left( \frac{2\mu + \omega}{q} \right) \right.$$

$$\left. + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{q^2 - (2\mu + \omega)^2} - (2\mu + \omega) \sqrt{q^2 - \omega^2}}{\omega \sqrt{q^2 - (2\mu + \omega)^2} - (2\mu + \omega) \sqrt{q^2 - \omega^2}} \right| \right]$$

$$+ \frac{g}{16\pi} \Theta(\omega - q) \Theta(|2\mu - \omega| - q) \times \left[ |2\mu - \omega| \sqrt{\frac{(2\mu - \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} \ell_n \left| \frac{q}{|2\mu - \omega| + \sqrt{(2\mu - \omega)^2 - q^2}} \right| \right.$$

$$\left. - \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{(2\mu - \omega)^2 - q^2} + |2\mu - \omega| \sqrt{\omega^2 - q^2}}{\omega \sqrt{(2\mu - \omega)^2 - q^2} - |2\mu - \omega| \sqrt{\omega^2 - q^2}} \right| \right]$$

$$+ \frac{g}{16\pi} \Theta(\omega - q) \times \left[ -(2\mu + \omega) \sqrt{\frac{(2\mu + \omega)^2 - q^2}{\omega^2 - q^2}} + \frac{3q^2 - 2\omega^2}{\sqrt{\omega^2 - q^2}} \ell_n \left| \frac{2\mu + \omega + \sqrt{(2\mu + \omega)^2 - q^2}}{q} \right| \right.$$

$$\left. + \frac{\omega^2 - q^2}{\omega} \ell_n \left| \frac{\omega \sqrt{(2\mu + \omega)^2 - q^2} + (2\mu + \omega) \sqrt{\omega^2 - q^2}}{\omega \sqrt{(2\mu + \omega)^2 - q^2} - (2\mu + \omega) \sqrt{\omega^2 - q^2}} \right| \right] .$$

(6.79)

This is plotted in Fig. 6.7 with cuts along different $\omega$ and $q$ in Figs. 6.8 and 6.9, respectively.

The most significant difference between the real part of the dice polarizability (Eq. (6.79)) and the graphene polarizability (Eq. (6.2)) is the logarithmic divergence at $\omega = \mu$ (seen in Fig. 6.7). This comes from the logarithmic term in the first line of the result in Eq. (6.79) and indicates a large amount of screening at that energy. This is the exact energy that separates the Fermi level from the highly degenerate flat band.

As with the imaginary part, a series of manipulations can take the expression for the dice
polarizability (Eq. (6.79)) to that of graphene (Eq. (6.2)). First, the logarithmic divergence in the first line is omitted. Further, the lengthy logarithmic term proportional to \((\omega^2 + q^2)/\omega\) in each of the large square brackets is omitted and the \(3q^2 - 2\omega^2\) factor on the second term in each bracket is replaced by \(q^2\).

Equipped with the polarizability function for the dice lattice, it is now possible to analyze the screening effects in this system. A renormalized Coulomb potential via Eqs. (2.37) and (2.50) allows for a more accurate description of the interaction between charge carriers in the system. Also, collective phenomena can be analyzed (next section), which are significantly affected by the large screening provided by the flat band. These ends could have been achieved through numerical evaluation of the polarizability. However, the analytical derivation performed in this chapter provides a much stronger insight into the fundamental entity of polarizability. By performing this derivation, explicit behaviours in the polarizability can be traced back to their fundamental origin in band structure dynamics.
Figure 6.8: Real part of the dice polarizability function along $q$ for four different values of $\omega$. The cuts in panels (b) and (c) are respectively situated on either side of the logarithmic divergence at $\omega = \mu$. Note that the positive divergence to the right of $q = \omega$ is too narrow to be shown in the first three panels.
Figure 6.9: Real part of the dice polarizability function along $\omega$ for four different values of $q$. Note that the positive divergence to the left of $\omega = q$ is too narrow to be shown in panel (a).
6.3 Screening Effects in the Dice Lattice

Plasmons

Equation (2.58) gives a formula allowing for the solution of the plasmon dispersion $\omega_p(q)$, which applies for a negligible plasmon scattering rate, $\eta_p$. Since the leading-order term in $\eta_p$ is proportional to $\text{Im} \, Q$ (Eq. (2.59)), Eq. (2.58) for $\omega_p$ is only accurate outside of the PHC. Inside the PHC, plasmon oscillations are heavily damped by particle-hole pair production.

In Fig. 6.10(c), the dice plasmon dispersion is plotted for varying values of the effective fine-structure constant, $\alpha$. Similar curves are given for graphene in panel (b) of the figure. In the DW systems, $\alpha = e^2/\epsilon_0 \hbar v$ is the ratio between the potential and kinetic energy of Dirac fermions (the dimensionless Wigner-Seitz radius [77,80]), representing the strength of the Coulomb potential. In a physical lattice, variation of $\alpha$ is achieved through replacement of the substrate, which provides the background dielectric constant, $\epsilon_0$ (graphene on SiO$_2$ has $\alpha \sim 0.5$ [77]).

The plasmon curves in Fig. 6.10 were constructed by graphical solution of Eq. (2.58) using $\text{Re} \, Q$ in Eq. (6.79). This procedure is demonstrated in Fig. 6.10(a) using a value of $\alpha = 0.5$. The curve $y_1 = -2\pi \alpha \text{Re} \, Q$ is plotted along $q$ for two example values of $\omega = 3\mu/4$ and $\omega = 0.999\mu \equiv \mu^-$ (blue and black, respectively). The intersection of $y_1$ with $y_2 = q$ (dashed red line) solves Eq. (2.58), marking a point in the plasmon energy dispersion, $(q, \omega_p)$.

In Figs. 6.10(b) and (c), the PHC for graphene and the dice lattice, respectively, is shaded in grey. Although the plasmon dispersions shown in the figure extend into the PHC, in reality Eq. (2.58) only applies outside of the PHC. A better visualization of the plasmon dispersion is in the loss function, $\text{Im} \, [1/\epsilon]$.

The differential cross section for the inelastic scattering of fast-moving test charges passing through the material is proportional to the dielectric loss function [81]. As such, the technique of electron energy-loss spectroscopy measures this function by firing electrons through a material and observing the spectrum of energy and momentum loss through scattering events [82]. A divergence in the loss function traces out the resonant excitation of plasmons in the material.
Figure 6.10: (a) Graphical solution of Eq. (2.58). Black and blue curves show $2\pi\alpha \Re Q$ for two different values of $\omega$. Intersections with $y = q$ (red dashed lines) are indicated with arrows. (b) Plasmon dispersions in graphene for three values of $\alpha$, allowed to extend into the PHC (shaded grey). (c) Plasmon dispersions in the dice lattice for various $\alpha$, with the PHC shaded grey.
Figure 6.11: Dice lattice loss function for (a) $\alpha = 0.5$ and (b) $\alpha = 2$.

The loss function for the dice lattice is plotted in Fig. 6.11 for two different values of $\alpha$. This was calculated using Eqs. (2.50), (6.30), and (6.79), with

$$\text{Im} \left[ \frac{1}{\epsilon(q, \omega)} \right] = -\frac{\epsilon_i}{\epsilon_r^2 + \epsilon_i^2},$$

(6.80)

where $\epsilon_r$ and $\epsilon_i$ are the real and imaginary parts of the dielectric function, respectively. Outside of the PHC (where $\text{Im} Q = 0$ and thus $\epsilon_i = 0$) it was necessary to provide a small imaginary part (on the order of $10^{-3} \mu$) in order to give the plasmon dispersion some width (blue curves in each panel). As the plasmon curve enters the PHC above $\omega = \mu$ it no longer presents as a well defined peak, but instead has a broad width and thus a large scattering rate.

Interestingly, the dice plasmon curves in Figs. 6.10(c) and 6.11 all pinch in to the point $\omega_p = q = \mu$ before extending into the PHC. The curves in graphene, on the other hand, enter the PHC at higher energy with increasingly large $\alpha$ (Fig. 6.10(b)). Away from the pinch point at $\omega = q = \mu$, the dice plasmon dispersion matches the trajectory of the dispersion in graphene. In Fig. 6.12, the plasmon curves for graphene and the dice lattice are overlaid. This plot assumes that the Fermi velocity is the same in both systems, which need not be the case. At low $q$, the dice curves matches the $\omega_p \propto \sqrt{q}$ behaviour of the graphene curves.
Figure 6.12: Dice (solid) and graphene (dashed) plasmon dispersions for various values of \( \alpha \). The plot assumes the same Fermi velocity in both systems.

As the energy grows toward \( \omega = q \), the dice curves are pinched into \( \omega = q = \mu \). Allowed to extend to higher energies, the graphene and dice dispersions eventually coincide again. This pinch point in the dice plasmon curve shows a significant difference to the behaviour in graphene. This feature is invariant to a change in the background dielectric (change in \( \alpha \)) and is a direct result of the singular density of states found in the flat band.

At the energy \( \omega = \mu \), \( \text{Re} Q \) in the dice lattice diverges to infinity as a result of the large screening from the flat band. As such, \( |\epsilon| \to \infty \) at this energy (Eq. (2.50)), meaning that plasmons cannot exist (since the criteria for their existence is a zero in the dielectric function, Eq. (2.56)). Equivalently, the loss function, \( \text{Im} [1/\epsilon] \), is exactly zero at \( \omega = \mu \) (Fig. 6.11). For any value of \( \alpha \), a plasmon is not allowed to exist at \( \omega_p = \mu \). Instead, the plasmon curve at this energy pinches into the most resonant part of the particle-hole scattering, at \( \omega = q \). That is, rather than a plasmonic excitation, a particle-hole pair is created in which the members of the pair are separated by energy \( \omega = \mu \) and momentum \( q = \mu \).
Friedel Oscillations

The polarizability, $Q$, is often referred to as the Lindhard function because it was Lindhard that first defined the object in 1954 (though he did not use the Green’s function method in its analysis) [83]. Instead of the general polarizability, $Q(q, \omega)$, we use ‘Lindhard function’ to refer to the static polarizability,

$$\mathcal{L}(q) = Q(q, 0),$$

which is an entirely real quantity.

The graphene and dice Lindhard functions both have a general form,

$$\mathcal{L}(q) = a(q) + \Theta(q - 2\mu)b(q),$$

which has a background term, $a$, existing for all $q$, and another term, $b$, which is only onset for $q > 2\mu$. In graphene [84],

$$a_g(q) = \frac{g}{2\pi}\mu,$$
$$b_g(q) = \frac{g}{8\pi} \left[ q \arccos \left( \frac{2\mu}{q} \right) - \frac{2\mu}{q} \sqrt{q^2 - 4\mu^2} \right],$$

while Eq. (6.79) gives the same in the dice lattice,

$$a_d(q) = \frac{g}{8\pi} \left( 4\mu + \frac{q^2}{\mu} \right),$$
$$b_d(q) = \frac{g}{8\pi} \left[ 3q \arccos \left( \frac{2\mu}{q} \right) - \left( \frac{2\mu}{q} + \frac{q}{\mu} \right) \sqrt{q^2 - 4\mu^2} \right].$$

For a regular 2D electron gas (2DEG), the chemical potential is not equal to the Fermi wavevector, $k_F$. As such, Eq. (6.82) gives the 2DEG Lindhard function after $\mu$ is generalized to $k_F$ [85], with

$$a_{eg}(q) = \frac{g}{2\pi}m,$$
$$b_{eg}(q) = \frac{g}{2\pi} \frac{m}{q} \sqrt{q^2 - 4k_F^2}.$$
Figure 6.13: Dice Lindhard function (black) showing constituent \(a\) (red dashed) and \(b\) (blue dashed) terms. Inset is the same for graphene.

The dice Lindhard function (Eq. (6.84)) is plotted in Fig. 6.13 as a black curve showing the constituent \(a\) (red dashed) and \(b\) (blue dashed) contributions. Inset in the figure is the same for graphene. Of note is that at the momentum \(q = 2\mu\) (\(q = 2k_F\) in the 2DEG), the Lindhard function is singular in its first, second, and third derivative in the 2DEG, graphene, and dice systems, respectively.

The Lindhard function, \(\mathcal{L}(q)\), allows for the determination of responses in the system to external electrostatic distributions. For example, if a point charge \(Q\) is introduced at a position \(\mathbf{r} = 0\), the potential around it is proportional to the Fourier transform of the renormalized Coulomb potential,

\[
\varphi(\mathbf{r}) = \frac{Q}{\alpha\epsilon_0} \int \frac{d^2q}{(2\pi)^2} \frac{V_c(q)}{\varepsilon(q)} e^{-iq \cdot \mathbf{r}} = \frac{Q}{\epsilon_0} \int_0^\infty dq J_0(qr) \frac{e^{-iq \cdot \mathbf{r}}}{\varepsilon(q)},
\]

(6.86)

where \(J_0\) is the zeroth Bessel function of the first kind.

The leading-order contribution to the screened potential is the Thomas-Fermi decay
Table 6.1: Decay in the screening potential around electromagnetic impurities in three different systems, showing the spatial behaviour of the Thomas-Fermi (TF) decay and the Friedel oscillations.

<table>
<thead>
<tr>
<th>System</th>
<th>TF</th>
<th>Friedel</th>
</tr>
</thead>
<tbody>
<tr>
<td>2DEG</td>
<td>$1/r^3$</td>
<td>$\sin(2k_F r)/r^2$</td>
</tr>
<tr>
<td>Graphene</td>
<td>$1/r^3$</td>
<td>$\sin(2\mu r)/r^3$</td>
</tr>
<tr>
<td>Dice</td>
<td>$1/r^3$</td>
<td>$\sin(2\mu r)/r^4$</td>
</tr>
</tbody>
</table>

(TF). Each of the three systems (2DEG, graphene, and dice) exhibits a $1/r^3$ spatial dependence in the TF decay. At next-to-leading order, an oscillatory decay occurs, referred to as Friedel oscillations. The rate of decay depends on the singular behaviour of each system at $q = 2\mu$ ($q = 2k_F$ in the 2DEG) [86]. In the 2DEG, the first derivative is singular, which leads to a $1/r^2$ decay in its Friedel oscillations. In graphene, it is the second derivative which is singular, leading to a faster rate of decay, $1/r^3$. This trend continues in the dice lattice where the singular third derivative gives a decay rate that goes as $1/r^4$.

Friedel oscillations are also seen in the induced spin structure around a magnetic impurity (but without any TF decay) [76]. This induced magnetic potential is also responsible for the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between two magnetic impurities. The strength of the RKKY interaction is proportional to the Fourier transform of the Lindhard function itself,

$$L(r) = \int \frac{d^2 q}{(2\pi)^2} L(q) e^{-iq \cdot r}$$

$$= \frac{1}{2\pi} \int_0^\infty q dq J_0(qr) L(q). \quad (6.87)$$

The TF and Friedel oscillation decay rates for each system are summarized in Table 6.1 and derived explicitly for the dice lattice below. First, the Friedel oscillations around a magnetic impurity are derived from Eq. (6.87). The Lighthill theorem states that the asymptotic behaviour of a Fourier-transform (i.e., large $r$-behaviour in $L(r)$) is dominated by singular behaviour in its integrand or any of the integrand’s derivatives. The singularity in the third derivative of $L(q)$ can be pieced out using integration by parts.
At large distances, as \( r \to \infty \),

\[
J_0(qr) \approx \frac{2}{\sqrt{2\pi qr}} \cos \left( qr - \frac{\pi}{4} \right) + O(r^{-3/2}). \tag{6.88}
\]

As we are only interested in the behaviour in \( r \) at long distances, the \( \pi/4 \) phase shift is disregarded. Then,

\[
\mathcal{L}_d(r) = \frac{1}{\pi \sqrt{2\pi r}} \int_0^\infty dq \sqrt{q} \cos(qr) \mathcal{L}_d(q). \tag{6.89}
\]

Making a change of variables to \( x = q - 2\mu \),

\[
\mathcal{L}_d(r) = \frac{1}{\pi \sqrt{2\pi r}} \int_{-2\mu}^{\infty} dx \sqrt{x + 2\mu} \cos[(2\mu + x)r] \mathcal{L}_d(2\mu + x). \tag{6.90}
\]

Since the singular behaviour (and main contribution to the integral) is about \( q = 2\mu \), it is fine to consider \( x \sim 0 \) and pull out a factor of \( \sqrt{2\mu} \) from the integrand. The cos factor is left inside the integral to aid with integration by parts which pulls out the third derivative \( \mathcal{L}^{(3)}_d(q) \) in the integrand. The boundary terms are discarded, so that after three integrations by parts,

\[
\mathcal{L}_d(r) = \frac{1}{\pi \sqrt{2\pi r}} \int_{-2\mu}^{\infty} dx \cos[(2\mu + x)r] \mathcal{L}_d(2\mu + x)
= -\frac{\sqrt\mu}{\pi^{3/2} r^{7/2}} \int_{-2\mu}^{\infty} dx \sin[(2\mu + x)r] \mathcal{L}^{(3)}_d(2\mu + x). \tag{6.91}
\]

From Eq. (6.84),

\[
\mathcal{L}^{(3)}_d(q) = -\frac{24\mu^3 \Theta(q - 2\mu)}{\pi q^4 \sqrt{q^2 - 4\mu^2}}
= -\frac{24\mu^3 \Theta(x)}{\pi (2\mu + x)^4 \sqrt{x(4\mu + x)}}
\approx -\frac{3 \Theta(x)}{4\pi \mu^{3/2} \sqrt{x}}, \quad x \sim 0. \tag{6.92}
\]
Using the technique developed by Lighthill [86], we write

\[
\mathcal{L}_d(r) = \frac{3}{4\pi^{5/2} \mu r^{7/2}} \sin(2\mu r) \int_{-\infty}^{\infty} \frac{dx}{\sqrt{x}} \Theta(x) \sqrt{x} = \frac{3}{8\pi^{5/2} \mu r^{7/2}} \sin(2\mu r) \int_{-\infty}^{\infty} \frac{dx}{|x|^{1/2}} \sqrt{|x|} = \frac{3 \sin(2\mu r)}{2\sqrt{2\pi^{2} \mu r^4}}.
\]

(6.93)

This gives the result reported in Table 6.1.

Each of the three integrations by parts performed in Eq. (6.91) pulled a factor of \(1/r\) out of the integral. In the same calculation for the 2DEG or graphene, fewer integrations by parts are necessary in order to piece out the singular behaviour in the integrand. As such, the Friedel oscillations have slower decay rates in these systems when compared to the dice lattice.

A similar calculation gives the dice Friedel oscillations in the electric potential via Eq. (6.86),

\[
\varphi_d(r) = -\frac{3\sqrt{2\alpha} Q}{32\epsilon_0(1 + 10\alpha)^2 \mu^3} \frac{\sin(2\mu r)}{r^4} \quad \text{(Friedel)}.
\]

(6.94)

The TF decay in \(\varphi_d(r)\) comes from the long-wavelength limit of the Lindhard function \((q \to 0)\),

\[
\mathcal{L}(q) = \frac{q}{8\pi} (4\mu + 6q) + \mathcal{O}(q^2).
\]

(6.95)

Then

\[
\frac{V_c(q)}{\epsilon(q)} = \frac{2\pi\alpha}{(1 + 6\alpha)q + q_{TF}} \approx \frac{2\pi\alpha}{q_{TF}} \left[1 - (1 + 6\alpha) \frac{q}{q_{TF}}\right].
\]

(6.96)

where \(q_{TF} = 4\alpha\mu\) is the TF wavevector in both the dice lattice and in graphene. Taking the Fourier transform of Eq. (6.96) gives the TF decay around a charge impurity in the dice lattice,

\[
\varphi_d(r) = \frac{2(1 + 6\alpha)\pi^2 Q}{q_{TF} \epsilon_0 r^3} \quad \text{(TF)}.
\]

(6.97)

Plasmonic behaviour and electrostatic potentials are just two examples of the collective
behaviour that can be analyzed using the dynamic polarizability function derived in this chapter. The polarizability (or equivalently the dielectric function) contains essentially all of the electronic information on the behaviour of free charge carriers, making it a very versatile, useful, and insightful tool in the study of this condensed matter system.
Chapter 7

Conclusions

This thesis has focused on electronic response functions of interesting relativistic condensed matter systems. These response functions (defined in Chapter 2) determine the susceptibility of a system to external probes. As such, they are of fundamental importance to experiment. A response function is an intrinsic property of the system under study. It does not depend on the specifics of an external stimulus, but rather the unique properties of the system. By determining the behaviour of a response function from experimental data, one can learn much about the microscopic physics giving rise to the material’s properties. From another point of view, by predicting the behaviour of a response function, one can identify experimental signatures for different classes of materials.

Excitement surrounding graphene (the $s = 1/2$ DW material) motivates the search for other novel relativistic materials. Chapter 3 details the various materials studied in this thesis and their properties, focusing on the role of pseudospin. Analyzing response functions in these materials can aid with their identification by experimentalists. In addition, the response functions provide a good deal of information on the dynamics in a system, more than band structure alone can reveal.

Chapters 4 and 5 derive the magneto-optical conductivity of general pseudospin-$s$ DW fermions and Kane fermions, respectively. Unique signatures are found in various optical spectra which act to identify each system. They also provide clear evidence for the relation between Kane and DW fermions as ‘relativistic’ particles because of similarities in these signatures. Specifically, analysis shows that a massless Kane fermion (restricted to 2D) is a hybrid $s = 1/2$ and $s = 1$ DW fermion. The invention of snowshoe diagrams aids
in the analysis of these spectra. Insight gained from a simplified model of Kane fermions was applied to the calculation of the absorbance spectrum of MCT from an extended Kane model.

The final piece of work in the thesis focused specifically on the $s = 1$ DW system with the full derivation of the dynamical polarizability in Chapter 6. This fundamental quantity influences the material’s dielectric function, which in turn renormalizes the Coulomb potential. From the polarizability, the plasmonic behaviour in the $s = 1$ system was analyzed along with the behaviour of Friedel oscillations around some electronic impurity. These are only two examples of the collective behaviour that can be determined via the polarizability. Another example is in polariton excitations. These arise from couplings between electromagnetic radiation and the material’s plasma (rather than a pure excitation of the plasma like for a plasmon) [34]. The polarizability of systems with yet-higher values of pseudospin could also be studied in the future. Each will have their own extensions of the particle-hole continuum compared to the basic $s = 1/2$ system due to the addition of more conic bands giving the possibility of more scattering events.

A major element of the thesis focused on the flat band found in the integer-pseudospin DW system and the Kane model. This highly degenerate band was assumed to be inert in all of the analyses made. The mere presence of it in the $s = 1$ system was shown in Chapter 6 to provide a large amount of screening at an energy equal to the chemical potential. In addition, its unique LL structure (with the absence of any LL at even values of Fock number $n < 2s$) creates recognizable signatures in optical spectra (Chapters 4 and 5). In addition, allowing for the possibility of interactions within the flat band could give rise to some rather interesting physics.

In the Bardeen-Cooper-Schrieffer theory of superconductivity, attractive interactions between degenerate electrons at the Fermi surface leads to the binding of Cooper pairs which then condense into the macroscopic superconducting quantum state [87]. Elsewhere, partial filling of LL’s in a 2DEG allows for special interactions that give rise to the fractional quantum Hall effect (FQHE) [48]. It may prove fruitful to consider interactions within the flat band found in many relativistic materials. A single LL has a large density of states, which allows for the FQHE. This causes one to consider the novel effects which may arise
from having a huge array of degenerate partially filled LL's in the flat band under the presence of a magnetic field.
Appendix A

Standard Integrals

Derivation of the dynamical polarizability function in Chapter 6 requires the identity of several angular integrals. These integrals, which depend on real parameters $a$ and $b$, are derived here in this appendix.

Integral $A_1$

The first of the standard integrals is

$$A_1 = \int_{-\pi}^{\pi} \mathcal{P} \frac{d\theta}{a - \cos \theta},$$

(A.1)

where $\mathcal{P}$ indicates integration over the principal part (Eq. (2.22)). A change of variables is made so that this becomes a closed integral in the complex $z$-plane, where $z = e^{i\theta}$. In this way, $d\theta = dz/i$ and the contour traces out the unit circle, $|z| = 1$. Then the integral is now written

$$A_1 = \oint_{|z|=1} \mathcal{P} \frac{dz}{iz} \frac{1}{a - \frac{1}{2}(z + \frac{1}{z})}$$

$$= \frac{-2}{i} \oint_{|z|=1} \mathcal{P} \frac{dz}{z^2 - 2az + 1}$$

$$= \frac{-2}{i} \oint_{|z|=1} \mathcal{P} \frac{dz}{(z - \zeta_+)(z - \zeta_-)},$$

(A.2)

where the two simple poles in the integrand are $\zeta_{\pm} = a \pm \sqrt{a^2 - 1}$. 

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Two broad cases arise based on the value of $a$,

- $a^2 > 1$: Both poles lie on the real axis. If $a > 1$, then $\zeta_-$ is contained by the contour while $\zeta_+$ lies outside of it (vice versa for $a < 1$).

- $a^2 < 1$: Here both poles are off of the real axis and are exactly on the unit circle $|\zeta|$. Because $A_1$ is defined to be an integral over the principal part, these poles (which lay on the contour of integration) are neglected.

Then, according to Cauchy’s residue theorem (and referring to the integrand as $f(z)$),

$$A_1 = -4\pi \left[ \Theta(a-1) \text{Res} f(\zeta_-) + \Theta(a+1) \text{Res} f(\zeta_+) \right]$$

$$= -4\pi \left( \frac{\Theta(a-1)}{\zeta_- - \zeta_+} + \frac{\Theta(a+1)}{\zeta_+ - \zeta_-} \right)$$

$$= 2\pi \left( \frac{\Theta(a-1)}{\sqrt{a^2-1}} - \frac{\Theta(a+1)}{\sqrt{a^2-1}} \right)$$

$$= \frac{2\pi}{\sqrt{a^2-1}} \text{sgn}(a) \Theta(a^2-1). \tag{A.3}$$

**Integral $A_2$**

The next integral is solved quickly,

$$A_2 = \int_{-\pi}^{\pi} d\theta \mathcal{P} \frac{\cos \theta}{a - \cos \theta}$$

$$= \int_{-\pi}^{\pi} d\theta \mathcal{P} \left( \frac{\cos \theta - a}{a - \cos \theta} + \frac{a}{a - \cos \theta} \right) \tag{A.4}$$

$$= -2\pi + aA_1$$

$$= -2\pi + \frac{2\pi a}{\sqrt{a^2-1}} \text{sgn}(a) \Theta(a^2-1).$$

**Integral $A_3$**

Next is the solution of

$$A_3 = \int_{-\pi}^{\pi} \mathcal{P} \frac{d\theta}{\cos^2 \theta + a \cos \theta + b}. \tag{A.5}$$
With a change of variables to \( z = e^{i\theta} \),

\[
A_3 = \oint \frac{dz}{iz} \frac{1}{\frac{1}{4}(z + \frac{1}{z})^2 + \frac{a}{2}(z + \frac{1}{z}) + b}
\]

\[
= \frac{4}{i} \oint dz P \frac{z}{z^4 + 2az^3 + 2(2b + 1)z^2 + 2az + 1}
\]

\[
= \frac{4}{i} \oint dz P \frac{z}{(z - \zeta_1)(z - \zeta_2)(z - \zeta_3)(z - \zeta_4)},
\]

where the integrand is written in terms of four simple poles

\[
\zeta_1 = \frac{1}{2} \left[ -a - \sqrt{a^2 - 4b} - \sqrt{2(a^2 - 2b - 2 + a\sqrt{a^2 - 4b)}} \right],
\]

\[
\zeta_2 = \frac{1}{2} \left[ -a - \sqrt{a^2 - 4b} + \sqrt{2(a^2 - 2b - 2 + a\sqrt{a^2 - 4b)}} \right],
\]

\[
\zeta_3 = \frac{1}{2} \left[ -a + \sqrt{a^2 - 4b} - \sqrt{2(a^2 - 2b - 2 - a\sqrt{a^2 - 4b})} \right],
\]

\[
\zeta_4 = \frac{1}{2} \left[ -a + \sqrt{a^2 - 4b} + \sqrt{2(a^2 - 2b - 2 - a\sqrt{a^2 - 4b})} \right].
\]

Evaluating the residues, the principal-part contour integration yields

\[
A_3 = 8\pi \left[ \frac{\zeta_1 \Theta(1 - |\zeta_1|)}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \frac{\zeta_2 \Theta(1 - |\zeta_2|)}{(\zeta_2 - \zeta_1)(\zeta_2 - \zeta_3)(\zeta_2 - \zeta_4)} 
\right.

\[
+ \frac{\zeta_3 \Theta(1 - |\zeta_3|)}{(\zeta_3 - \zeta_1)(\zeta_3 - \zeta_2)(\zeta_3 - \zeta_4)} + \frac{\zeta_4 \Theta(1 - |\zeta_4|)}{(\zeta_4 - \zeta_1)(\zeta_4 - \zeta_2)(\zeta_4 - \zeta_3)} \right].
\]

The solution is left in this form rather than expanding it out in terms of \( a \) and \( b \). In

Chapter 6 where these integrals are employed, it is simpler to use the \( \zeta \)'s.

**Integral \( A_4 \)**

Next is

\[
A_4 = \int_{-\pi}^{\pi} d\theta P \frac{\cos \theta}{\cos^2 \theta + a \cos \theta + b}.
\]
Changing variables to $z = e^{i\theta}$,

$$A_4 = \oint P \frac{dz}{iz} \left[ \frac{1}{4} (z + \frac{1}{z})^2 + \frac{a}{2} (z + \frac{1}{z}) + b \right]$$

$$= \frac{2}{i} \oint dz P \frac{z^2 + 1}{(z - \zeta_1)(z - \zeta_2)(z - \zeta_3)(z - \zeta_4)}$$

$$= 4\pi \left[ \frac{(\zeta_1^2 + 1) \Theta(1 - |\zeta_1|)}{(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \frac{(\zeta_2^2 + 1) \Theta(1 - |\zeta_2|)}{(\zeta_2 - \zeta_1)(\zeta_2 - \zeta_3)(\zeta_2 - \zeta_4)} + \frac{(\zeta_3^2 + 1) \Theta(1 - |\zeta_3|)}{(\zeta_3 - \zeta_1)(\zeta_3 - \zeta_2)(\zeta_3 - \zeta_4)} + \frac{(\zeta_4^2 + 1) \Theta(1 - |\zeta_4|)}{(\zeta_4 - \zeta_1)(\zeta_4 - \zeta_2)(\zeta_4 - \zeta_3)} \right]. \tag{A.10}$$

**Integral $A_5$**

The second-to-last integral is

$$A_5 = \int_{-\pi}^{\pi} d\theta P \frac{\cos^2 \theta}{\cos^2 \theta + a \cos \theta + b}. \tag{A.11}$$

Mapping this onto a contour integral in the complex plane,

$$A_5 = \oint dz P \frac{1}{4} \left( z + \frac{1}{z} \right)^2 + \frac{a}{2} \left( z + \frac{1}{z} \right) + b$$

$$= \frac{1}{i} \oint dz P \frac{z(z - \zeta_1)(z - \zeta_2)(z - \zeta_3)(z - \zeta_4)}{(z^2 + 1)^2} \tag{A.12}$$

$$= 2\pi \left[ 1 + \frac{(\zeta_1^2 + 1)^2 \Theta(1 - |\zeta_1|)}{\zeta_1(\zeta_1 - \zeta_2)(\zeta_1 - \zeta_3)(\zeta_1 - \zeta_4)} + \frac{(\zeta_2^2 + 1)^2 \Theta(1 - |\zeta_2|)}{\zeta_2(\zeta_2 - \zeta_1)(\zeta_2 - \zeta_3)(\zeta_2 - \zeta_4)} + \frac{(\zeta_3^2 + 1)^2 \Theta(1 - |\zeta_3|)}{\zeta_3(\zeta_3 - \zeta_1)(\zeta_3 - \zeta_2)(\zeta_3 - \zeta_4)} + \frac{(\zeta_4^2 + 1)^2 \Theta(1 - |\zeta_4|)}{\zeta_4(\zeta_4 - \zeta_1)(\zeta_4 - \zeta_2)(\zeta_4 - \zeta_3)} \right].$$

**Integral $A_6$**

This last integral can be written in terms of the first one,

$$A_6 = \int_{-\pi}^{\pi} d\theta P \frac{\sin^2 \theta}{a + \cos \theta}$$

$$= \int_{-\pi}^{\pi} d\theta P \left( \frac{a^2 - \cos^2 \theta}{a + \cos \theta} + \frac{1 - a^2}{a + \cos \theta} \right)$$

$$= \int_{-\pi}^{\pi} d\theta (a - \cos \theta) + (1 - a^2) \int_{-\pi}^{\pi} P \frac{d\theta}{a + \cos \theta}$$

$$= 2\pi a - 2\pi \sqrt{a^2 - 1} \text{sgn}(a) \Theta(a^2 - 1). \tag{A.13}$$
Bibliography


