The Dimensionless Kadowaki-Woods Ratio in Arbitrary Band Structures and Two Dimensional Graphene

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DECLARATION

This thesis is an account of research undertaken between July 2013 and June 2014 in the Department of Physics, School of Maths and Physics, Faculty of Science, at the University of Queensland, Australia under the supervision of Associate Professor Ben Powell and Dr Anthony Jacko.
Except where acknowledged, the material presented here is, to the best of my knowledge, original and has not been submitted in whole or part for a degree in any university.

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ABSTRACT

Fermi liquid theory describes the normal state of most metallic materials with unparalleled accuracy [1–9]. A small but growing number of materials exist, however, that are not described by Fermi liquid theory [10–19]. These non-Fermi liquids are characterised by unusual transport and thermodynamic properties, many of which present not only a challenge to theoretical models, but also the potential for numerous applications. As of yet, however, many non-Fermi liquid states are difficult, if not impossible, to confirm experimentally. As such, experimental signatures of non-Fermi liquid behaviour are needed to definitively identify non-Fermi liquid materials.

A divergence of the Kadowaki-Woods ratio has been proposed as a possible experimental probe of non-Fermi liquid behaviour. In the dimensionless form derived by Jacko, Fjærestad and Powell, the Kadowaki-Woods ratio takes a near-universal value in a wide range of Fermi-liquid systems, and unusual values may be indicative of non-Fermi liquid behaviour [20]. Before this can be implemented as a test of Fermi liquid behaviour, however, the ratio must be generalised to incorporate band structure effects neglected in its original derivation, which may also give rise to divergent behaviour. The generalisation of the dimensionless Kadowaki-Woods ratio to include band structure effects forms the focus of this work. We find that the effects of arbitrary band structures can be taken into account by combining the material-specific parameters for the individual bands in a straightforward manner. Implementing the results of this generalisation can then be performed computationally, using density functional theory or some equivalent band structure determination method to calculate these material-specific quantities. Due to the complexity of such a calculation, the remainder of this work focuses on investigating the value of this generalised ratio, as well as the effects of reduced dimensionality, in monolayer graphene, for which the band structure effects are, at low energies, analytically tractable. We find that the Kadowaki-Woods ratio in graphene depends quadratically on the electron density, which can be controlled externally, presenting a potential test of the behaviour of the dimensionless ratio at extremely low electron densities. We then calculate the effects of the reduced dimensionality of graphene on the Kadowaki-Woods ratio, and find that for a model self-energy, the ratio gains an additional constant factor, and so, in principle, the effects of reduced dimension on the self-energy and resistivity may potentially be indirectly testable via the dimensionless Kadowaki-Woods ratio.
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1. INTRODUCTION

In this chapter, we give a brief overview of Fermi liquid theory, and why the Kadowaki-Woods ratio is an important consequence of it. In the following chapter, we then present a generalisation of the dimensionless Kadowaki-Woods ratio to systems of arbitrary band structure, which is applied to monolayer graphene in Chapters 3 to 5.

1.1 Fermi Liquid Theory

Attempts to explain and predict the electronic properties of solids began with Drude, who, with the discovery of the charge-carrying electron, attempted to describe the transport properties of metals by assuming that electrons in a material acted as an ideal classical gas, with no interactions [3]. By using the kinetic theory of gases, Drude made several accurate predictions, including the universality of the Wiedemann-Franz law (a constant empirical ratio between the electrical and thermal conductivities), and the form of the electrical conductivity. However, the heat capacity calculated according to Drude’s theory is temperature independent (as opposed to the observed linear temperature dependence) and the quadratic temperature dependence of the resistivity, the dominant contribution at low temperatures, is not explained by the theory [3].

Sommerfeld later improved upon Drude’s theory by treating the electrons quantum mechanically, using Fermi-Dirac statistics, while still assuming interactions between electrons were negligible [3]. As a result, the Drude-Sommerfeld free electron model correctly predicted the linear temperature dependence of the heat capacity, but with a coefficient that differed, sometimes considerably, in magnitude from measured values. The origin of the temperature dependence of the resistivity, however, remained unexplained by the free electron model, as did the reason why the heat capacity obeyed a non-interacting relationship, despite interactions between electrons being of considerable strength in many materials. It was not until the formulation of Fermi liquid theory, that the temperature dependence of the heat capacity could be accurately predicted and the origin of the temperature dependence of the resistance explained.

In the 1950’s, Landau first formulated his theory of the Fermi liquid [1, 2], to explain the measured properties of the liquid phase of Helium-3 in terms of the system’s low-energy excitations. Fermi liquid theory has since become an indispensable tool for studying the properties of interacting Fermi systems, in particular the properties of electrons in strongly correlated materials. Landau’s theory is based on the assumption of adiabatic continuity, that the interacting system can be generated from the equivalent non-interacting system by adiabatically turning on the interactions (see Fig. 1.1 for a representation of the adiabatic process). The adiabaticity of the process ensures that the quantum numbers of the non-interacting eigenstates (e.g. spin and momentum for a free fermion gas) are unchanged by the interactions, while the dynamical properties such as the energy, mass and velocity may be renormalized. In the interacting system, the quantum numbers no longer refer to the strongly interacting particles themselves, but weakly interacting quasiparticles consisting of the bare particles and the collected effects of their interactions with the surrounding particles. The collective dynamics of the system of weakly interacting quasiparticles can then be calculated using the well-known methods of statistical mechanics, and many of the difficulties of dealing with a complex interacting problem bypassed. Additionally, the weak remnant quasiparticle-quasiparticle interactions can be taken into account to explain properties that cannot be clearly understood from a non-interacting perspective. Chief among such properties are the quadratic temperature dependence of the electrical resistivity of metals at low temperatures, which is explained in Fermi liquid theory as the result of electron-electron scattering[7].

At low temperatures, Fermi liquid theory predicts the resistivity, $\rho(T)$, to obey the observed relationship

$$\rho(T) = \rho_0 + AT^2,$$

(1.1)

where $\rho_0$ is the zero temperature resistivity arising from impurity scattering and the quadratic term arises, in the Fermi liquid theory description, from electron-electron interactions. This quadratic dependence can be predicted by Fermi’s golden rule calculations of the weak quasiparticle-quasiparticle scattering [7, 21, 22]. Equivalently, the temperature dependence is contained in the imaginary part of the self-energy, which arises in the Kubo linear response formula for conductivity, in the many-body formalism outlined below [6].
1. Introduction

Fig. 1.1: Schematic of adiabatic continuity, for a potential $V(x) = \frac{1}{2} \lambda x^2$ inside the well and $V(x) = \infty$ outside. Starting from an infinite well potential, the ‘interaction,’ in this case a harmonic potential, is adiabatically turned on. As $\lambda$ increases gradually from 0 to 1, the energy of each state, as well as its exact form, are altered by the interaction, while the relevant quantum numbers, $N$, remain unchanged. Reproduced from [10].

Additionally, Fermi liquid theory triumphs in predicting the magnitude of the linear heat capacity coefficient, another failing of the models of Drude and Sommerfeld [3]. At low temperatures, the electronic heat capacity of a gas of weakly interacting fermions follows the relationship [3, 7]

$$C_{el} = \gamma T = \frac{m^* p_F^2 k_B^2 T}{3\hbar^3} = \frac{m^* m_0 p_F^2 k_B^2 T}{m_0 3\hbar^3} D_0(\varepsilon_0) = \frac{m^*}{m_0} \gamma_0 T,$$

(1.2)

where $m^*$ is the effective mass and $m_0$ is the bare (non-interacting) mass, $D_0(\varepsilon_0)$ is the bare density of states at the Fermi energy and $\gamma_0$ is the linear coefficient predicted by the non-interacting Sommerfeld theory (or Bloch theory, which describes electron states in terms of band parameters, rather than free electron states [3]). The effective mass predicted by Fermi liquid theory, which can vary considerably from the bare electron mass, depending on the strength and nature of the electron-electron interactions, accounts for the considerable deviations of measured values of $\gamma$ from $\gamma_0$. [21, 23–25]

Fermi liquid theory can be formulated in terms of many-body perturbation theory and the Green’s function (or propagator) for a single quasiparticle [5, 7]. Although this approach is challenging mathematically, it allows for the calculation of many Fermi liquid properties in a straightforward manner.

1.1.1 The Self-Energy

In a non-interacting system, the Green’s function describes the probability amplitude that a particle will propagate between two points in a given time period, given by [6]

$$G^{(0)}(\vec{x}, t; \vec{x'}, t') = -i \langle T_{t, t'} c_{\vec{x}}^\dagger(t') c_{\vec{x}}(t) \rangle,$$

(1.3)

where $T_{t, t'}$ is the time ordering operator, $c_{\vec{x}}^\dagger(t)$ and $c_{\vec{x}}(t)$ respectively create and annihilate a particle at time $t$ and position $\vec{x}$ and $\langle (...) \rangle$ denotes the average over the ground state of the system. In a periodic system, the Green’s function is generally only a function of the difference between the two points $\vec{x}$ and $\vec{x'}$ and the two times $t$ and $t'$, rather than the exact values of the
variables, so the Fourier transform in both variables is often used. The bare (non-interacting) single-particle Green’s function for a particle with energy $\omega$ and wavevector $\mathbf{k}$ is given by [6]

$$G_{\omega,\mathbf{k}}^{(0)} = \frac{1}{\omega - \varepsilon_{\mathbf{k}} + i\delta}$$  \hspace{1cm} (1.4)$$

where $\delta$ is the infinitesimal scattering rate ($\delta \to 0$ in the non-interacting case) and $\varepsilon_{\mathbf{k}}$ is the energy of the particle with wavevector $\mathbf{k}$, in the absence of electron-electron interactions.

The effect of interactions on the Green’s function can be taken into account via the self-energy, $\Sigma_{\omega,\mathbf{k}} = \Sigma'_{\omega,\mathbf{k}} + i\Sigma''_{\omega,\mathbf{k}}$, considered as the summation of ways in which the particle may interact with its environment, in the absence of vertex corrections, which renormalise the electron charge.

When calculating the effect of scattering on the single particle Green’s function, a sum is performed over the series of diagrams representing interactions with some scattering potential resulting from interaction with an impurity, electron or some other scattering mechanism [5, 26].

With diagrams defined by

$$= G_{\mathbf{k},\omega}^{(0)}; \hspace{1cm} = U \hspace{1cm} = G_{\mathbf{k},\omega};$$

with $G_{\mathbf{k},\omega}^{(0)}$ the bare Green’s function, $G_{\mathbf{k},\omega}$ the dressed (interacting) Green’s function and $U_{\mathbf{k}}$ the scattering potential. For ease of visualisation, we use here the impurity scattering potential, but the electron-electron scattering that forms the focus of this work can be recovered by replacing the electron-impurity interactions with electron-electron interactions.

$$G_{\mathbf{k},\omega} = G_{\mathbf{k},\omega}^{(0)} + G_{\mathbf{k},\omega}^{(0)} \Sigma_{\mathbf{k},\omega} G_{\mathbf{k},\omega},$$  \hspace{1cm} (1.5)$$

where $\Sigma_{\mathbf{k},\omega}$, the self-energy, is the sum of all irreducible terms in the series of diagrams, which represents the ways in which the particle may interact with itself and its environment, neglecting those given by vertex corrections [5]. The dressed Green’s function, containing all of the interactions characterised by the self-energy, is related to the bare Green’s function via Dyson’s equation (Eqn. (1.5)), which can be rearranged to give

$$G_{\omega,\mathbf{k}}^{-1} = \left(G_{\omega,\mathbf{k}}^{(0)}\right)^{-1} - \Sigma_{\omega,\mathbf{k}}$$ \hspace{1cm} (1.6)$$

$$G_{\omega,\mathbf{k}} = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma'_{\omega,\mathbf{k}} - i\Sigma''_{\omega,\mathbf{k}}},$$  \hspace{1cm} (1.7)$$

where the self-energy includes all of the particle interactions (where vertex corrections are neglected) and the resulting quasiparticle properties. On comparison with the non-interacting Green’s function, Eqn. (1.4), it can be seen that the imaginary part contributes to the quasiparticle scattering rate, resulting in a non-zero value, due to the interactions, while the real part can
be seen to be a shift in the quasiparticle energy. The quasiparticle scattering rate, $\frac{1}{\tau_{\omega,k}}$, upon which the resistivity depends, is related to the imaginary part of the self-energy by [5, 6]

$$\frac{1}{\tau_{\omega,k}} = -\frac{2\Sigma''_{\omega,k}}{\hbar},$$

while the energy renormalisation, characterised by the effective mass, $m^*$, arises from the shift in energy due to the real part of the self-energy, and is related to the self-energy and the bare mass $m_0$ via [5, 6]

$$\frac{m^*}{m_0} = \frac{v_0}{v^*} = \left[1 + \left(\frac{\partial}{\partial k}\right)^{-1} \frac{\partial \Sigma'_{\omega,k}}{\partial \omega} \right] k = k_F, \epsilon = \epsilon_F = 1 + (\frac{1}{v_0}) \frac{\partial \Sigma'_{\omega,k}}{\partial k} |_{k = k_F, \epsilon = \epsilon_F} Z = 1 + (\frac{1}{v_0}) \frac{\partial \Sigma'_{\omega,k}}{\partial k} |_{k = k_F, \epsilon = \epsilon_F} Z^{-1}.$$ (1.10)

### 1.1.2 The Kramers-Kronig Relations

As long as the self-energy is analytic in half of the complex plane and vanishes sufficiently fast as $\omega \to 0$ (properties guaranteed by causality), the real and imaginary parts of the self-energy are related by the Kramers-Kronig relations [27, 28]

$$\Sigma'_{\omega} = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\Sigma''_{\omega'}}{\omega' - \omega} d\omega',$$

$$\Sigma''_{\omega} = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\Sigma'_{\omega'}}{\omega' - \omega} d\omega',$$

where $P$ denotes the Cauchy principle value of the integral. The self-energy is known to obey these relations [6, 29], allowing the resistivity, a measure of how much energy is lost as heat when a current is passed through a material (which depends on the scattering rate (Eqn. (1.8))), and the heat capacity, a measure of how much energy is needed to raise the temperature of the material (which depends on the effective mass (Eqn. (1.10))), two quantities accurately predicted by Fermi liquid theory, to be related to one another. This is an example of a form of fluctuation-dissipation theorem, which relates the nonequilibrium linear response of a system to an external perturbation (in this case, the resistivity) to the fluctuations of the system at thermodynamic equilibrium (given here by the heat capacity) [30].

### 1.1.3 The Unitarity Limit of Scattering

The distinctive temperature dependence of the resistivity, as described by Fermi liquid theory, is known to arise from electron-electron scattering. In many of the following calculations we take the unitarity limit of the electron-electron scattering, corresponding to the upper bound on the scattering cross-section guaranteed by the unitarity of the scattering $S$-matrix [31]. The requirement of unitarity is a consequence of the need for the conservation of total probability in a realistic scattering process. For a spherically symmetric scattering potential, the potential and the incoming wave may be expanded in terms of spherical harmonics, and the restriction of probability conservation, combined with the symmetry of the scattering potential, implies that the scattering process cannot change the angular momentum of the incoming wave. As a result, not only is the total probability conserved, the probability for each partial wave is conserved. So, the scattering of the particle can result in at most a change of phase, $\delta_\ell$, for each of the partial waves with angular momentum $\ell$ [31]. The total cross-section is then, in three dimensions, [31]

$$\sigma_{3D} = \frac{4\pi}{k^2} \sum_\ell \sigma_\ell,$$ (1.12)

and in two dimensions, [32, 33]

$$\sigma_{2D} = \frac{4}{k} \sum_\ell \sigma_\ell,$$ (1.13)
where, in both cases, $\sigma_\ell$ is the partial wave cross section for the wave with angular momentum $\ell$,

$$\sigma_\ell = (2\ell + 1) \sin^2 \delta_\ell,$$

$k$ is the wavenumber of the incident particle and the sums are performed over all angular momentum states. If we assume incident $s$-waves (spherically symmetric, $\ell = 0$), and that $\sin^2 \delta_\ell$ assumes the maximum value possible, 1, we arrive at the maximum scattering cross-section, given by the unitarity limit

$$\sigma_{u;3D} = \frac{4\pi}{k^2},$$

$$\sigma_{u;2D} = \frac{4}{k}.$$ (1.14)

The scattering rate in a Fermi liquid (which is itself related to the imaginary part of the self energy via Eqn. (1.8)) is related to the scattering cross section by [8]

$$\frac{1}{\tau_{e-e}} = v_F n \sigma,$$ (1.15)

where $v_F$ is the average (Fermi) velocity of electrons and $n$ is the electron density. In the unitarity limit, the scattering rate becomes [20, 34]

$$\frac{1}{\tau_{e-e}} = \frac{\hbar n}{3\pi D_0 (\varepsilon_F)},$$ (1.16)

where $D_0 (\varepsilon_F)$ is the density of states at the Fermi energy. The characteristic energy scale ($s = \frac{\hbar}{2\tau_{e-e}}$) associated with this maximal scattering is of great importance in deriving the dimensionless Kadowaki-Woods ratio in Chapter 2 (see also Appendix A.1 for the derivation of the single band dimensionless Kadowaki-Woods ratio of Jacko, Fjærestad and Powell).

### 1.2 The Kadowaki-Woods Ratio

In 1968, Rice [35] observed that the coefficient of the quadratic term in the resistivity, $A$, should vary with the square of the linear heat capacity coefficient, $\gamma$. Rice further verified that, for a range of transition metals, the ratio of the two $\frac{A}{\gamma}$ was indeed constant, for measured values. Later, Kadowaki and Woods [36] found that in a variety of heavy fermion compounds, the ratio of the two measured quantities, which has since become known as the Kadowaki-Woods ratio (KWR), was again constant, though at a value approximately 25 times greater than that found in the transition metals.

Miyake, Matsuura and Varma (MMV) [34] later demonstrated that, if the self-energy can be said to be approximately constant with respect to the wavevector $k$, then the universality within material classes of the Kadowaki-Woods ratio is a direct consequence of the analytic properties of the electron self-energy, namely, the Kramers-Kronig relations, Eqn. (1.11). Using a phenomenological form for the self-energy, MMV recovered a value for the Kadowaki-Woods ratio in good agreement with that found in a range of heavy fermion compounds. MMV additionally claimed that the difference in the value of the Kadowaki-Woods ratio between different classes of material could be explained as a result of the varying strengths of the many-body correlations, and so the value of the ratio was proposed as a method for experimentally determining the strength of electronic interactions in a material.

Kontani [37] and later Tsuji, Kontani and Yoshimura [38] sought to explain the variations in the Kadowaki-Woods ratio as an effect of degeneracy, due to orbital angular momentum effects, with some success in heavy fermion compounds. Experimental findings by Li et al. in 2004 detected an anomalously large Kadowaki-Woods ratio in sodium cobaltate ($\text{Na}_{0.7}\text{CoO}_2$), which was considered, based on the work of MMV, to be indicative of strong electronic correlations [34, 39]. The authors claimed that the unusual value for the ratio was due to enhanced electron-electron scattering, evidence for the possible existence of a quantum critical point, or the proximity of a metal-insulator transition. Hussey [40], motivated by these, and other, anomalous Kadowaki-Woods ratio measurements, emphasized the importance of the units used to express both $A$ and $\gamma$ (which are usually given in volumetric and molar units, respectively) as well as the sensitivity of the ratio to material specific quantities, which also explain the unusually large Kadowaki-Woods ratio in $\text{Na}_{0.7}\text{CoO}_2$. Hussey also proposed differing forms of the Kadowaki-Woods ratio to account for the material’s dimension and the number of bands crossing the Fermi level to form sheets in the Fermi surface of the material, as well as suggesting that the ratio might be expressed in a dimensionless form.
1.2.1 The Dimensionless Kadowaki-Woods ratio

This suggestion, as well as the wide range of observed values in other materials (see Fig. 1.2), motivated Jacko, Fjærestad and Powell [20] to derive a dimensionless form of the Kadowaki-Woods ratio. This was accomplished by expanding on the work of MMV to include the influence of non-interacting material-specific quantities where MMV focused solely on the parameters of the interacting system and differing interaction strengths, an important difference highlighted by Hussey [40]. They determined that variations in the Kadowaki-Woods ratio were predominantly the result of these material specific quantities, rather than the strength of interactions, as proposed by MMV. Jacko, Fjærestad and Powell also demonstrated the approximately universal nature of this new dimensionless ratio across several classes of known Fermi liquid materials, including a wide selection of oxides and organic compounds, in addition to the transition metals and heavy fermion compounds (see Fig. 1.3). This dimensionless Kadowaki-Woods ratio is then, potentially, a useful experimental signature of the Fermi liquid state, unlike the dimensionful form of the ratio used by Li et al. [39].

The work of Jacko, Fjærestad and Powell demonstrated that, by taking into account the material-specific quantities, a new ratio, defined in terms of the Kadowaki-Woods ratio, can be found that takes a near universal value. As such, unusual values of the dimensionless ratio might be used as an experimental probe of non-Fermi liquid behaviour. This dimensionless Kadowaki-Woods ratio was derived, however, on the basis of a number of assumptions that may also lead to divergences in the measured value of the ratio. In particular, Jacko, Fjærestad and Powell derived their result for a material with a single band at the Fermi surface, obeying a parabolic (free electron) dispersion, as well as neglecting vertex corrections. As such, while a divergence of the dimensionless Kadowaki-Woods ratio could indicate non-Fermi liquid behaviour, it may also arise due to the invalidity of these assumptions. This work is focused on deriving a generalisation of the dimensionless Kadowaki-Woods ratio for systems with arbitrary band structure, extending the previously derived ratio to include systems with non-spherical Fermi surfaces and multiple bands crossing the Fermi level to form ‘sheets’ (or ‘pockets’) in the Fermi surface. The derivation of this generalised form of the Kadowaki-Woods ratio is the focus of Chapter 2, the results of which are, in principle, applicable to a wide variety of materials. The application of this generalised Kadowaki-Woods ratio to realistic materials is complicated in practice and requires significant modifications be made to existing computational electronic structure determination techniques (such as density functional theory). As a consequence, the remaining chapters concentrate on analysing the resulting relationship when applied to monolayer graphene, a two-dimensional semimetal which may be treated analytically without resorting to electronic structure calculations. Chapter 3 focuses on the straightforward application of the general relationship to graphene, while Chapters 4 and 5 take into account additional modifications to the generalised Kadowaki-Woods ratio due to contributions to the self-energy in two dimensions that are absent in three dimensional systems.
Fig. 1.3: Measured values of the dimensionless Kadowaki-Woods ratio for a variety of Fermi liquid materials, reproduced from [20].
2. THE KADOWAKI-WOODS RATIO IN ARBITRARY BAND STRUCTURES

In this chapter, we aim to generalise the result of Jacko, Fjærestad and Powell [20] to the case of arbitrary band structures. To achieve this, we first derive the form of the Green’s function in the two band case with arbitrary dispersion (the simplest example of a band structure with more than one band), then calculate the resistivity and heat capacity to determine the form of the dimensionless Kadowaki-Woods ratio. This general formulation will then be used in Chapter 3 to analyse the Kadowaki-Woods ratio in graphene, which possesses a Fermi surface of two identical ‘sheets,’ with a linear dispersion, and presents an interesting, and, importantly, analytically tractable (without the need for computational electronic structure calculations), example of the significance of including the band structure of a material in calculating the Kadowaki-Woods ratio.

2.1 Scattering and the Self-Energy

2.1.1 One Band Systems

Expressing the (in general, complex) self-energy for a one-band system as a sum of its real and imaginary parts \( \Sigma = \Sigma' + i\Sigma'' \)

\[
G_{k,\omega} = \frac{1}{\omega - \varepsilon_k - \Sigma'_{k,\omega} - i \left( \Sigma''_{k,\omega} - \delta \right)} = \frac{\omega - \varepsilon_k - \Sigma'_{k,\omega} + i \left( \Sigma''_{k,\omega} - \delta \right)}{\left( \omega - \varepsilon_k - \Sigma'_{k,\omega} \right)^2 + \left( \Sigma''_{k,\omega} - \delta \right)^2} = \frac{\eta_{k,\omega} + i\Gamma_{k,\omega}}{\eta_{k,\omega}^2 + \Gamma_{k,\omega}^2}\]

(2.1)

In the final line of Eqn. (2.1), we have defined the quantities

\[
\eta_{k,\omega} = \omega - \varepsilon_k - \Sigma'_{k,\omega}, \quad \Gamma_{k,\omega} = \Sigma''_{k,\omega} - \delta,
\]

(2.2)

(2.3)

which will become useful when considering the spectral density function \( A_{k,\varepsilon} = -2\text{Im} \{ G_{k,\omega} \} \) used in calculating the conductivity.

2.1.2 The Spectral Density Function (One Band)

In general, the dressed Green’s function can be expressed in terms of the spectral density function, \( A_{k,\varepsilon} \), [6]

\[
G_{k,\omega} = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \frac{A_{k,\varepsilon}}{\varepsilon - \omega + i\delta},
\]

(2.4)

and the spectral density function can be found from the Green’s function according to

\[
A_{k,\varepsilon} = -2\text{Im} \{ G_{k,\omega} \},
\]

(2.5)

which becomes, for the one-band case,

\[
A_{k,\varepsilon} = \frac{-2\Gamma_{k,\omega}}{\eta_{k,\omega}^2 + \Gamma_{k,\omega}^2}.
\]

(2.6)
Taking the limit as $\Gamma_{k,\omega} \to 0$, equivalent to the low energy limit of the system,

$$
\lim_{\Gamma_{k,\omega} \to 0} A_{k,\varepsilon} = \lim_{\Gamma_{k,\omega} \to 0} \frac{-2\Gamma_{k,\omega}}{\eta_{k,\omega}^2 + \Gamma_{k,\omega}^2} = -2\pi \delta (\eta_{k,\omega}). \tag{2.7}
$$

The low energy limit of the spectral density function squared $(A_{k,\varepsilon})^2$, is the quantity of interest in the conductivity derivation below. When integrated over all energies, the squared spectral density function, as defined in Eqn. (2.6), satisfies the integral relationship [6]

$$
\int_{-\infty}^{\infty} d\eta \frac{2\Gamma}{\eta^2 + \Gamma^2} = 1, \tag{2.8}
$$

which motivates expressing $(A_{k,\varepsilon})^2$ in the limiting case

$$
\lim_{\Gamma_{k,\omega} \to 0} (A_{k,\varepsilon})^2 = \lim_{\Gamma_{k,\omega} \to 0} \frac{4\Gamma_{k,\omega}^2}{(\eta_{k,\omega}^2 + \Gamma_{k,\omega}^2)^2} = \frac{2\pi \delta (\eta_{k,\omega})}{\Gamma_{k,\omega}}, \tag{2.9}
$$

which takes the desired value when integrated. At low energy, according to Eqn.(1.10), the real part of the self-energy can be approximated as

$$
\Sigma'_{k,\varepsilon} = (1 - Z^{-1}) \varepsilon, \tag{2.10}
$$

which gives, in terms of Eqns. (2.2) and (2.3)

$$
\lim_{\Gamma_{k,\omega} \to 0} (A_{k,\varepsilon})^2 = \frac{2\pi \delta (\eta_{k,\omega})}{\Gamma_{k,\omega}} = \frac{-2\pi \delta (\varepsilon - \varepsilon_k - (1 - Z^{-1}) \varepsilon)}{\Gamma_{k,\omega}}\nonumber = \frac{-2\pi \delta (Z^{-1} \varepsilon - \varepsilon_k)}{\Sigma'_{k,\omega}} = \frac{-2\pi Z \delta (\varepsilon - Z \varepsilon_k)}{\Sigma'_{k,\omega}}. \tag{2.11}
$$

In the calculation of the resistivity, the squared spectral density function appears in the Kubo formula for the conductivity and is of vital importance (see Appendix A.1, for the derivation of the resistivity in the one band case). Thus, the following sections are devoted to determining the form of the squared spectral density function in systems of more than one band.

2.1.3 Two Band Systems

In modelling scattering for more than one band, the Green’s function is a matrix, with the diagonal matrix elements giving the propagation in the bands (with energies given by the band dispersions), while the off-diagonal elements give the probability to propagate between bands. For our discussion, we begin with the simplest case, that of two bands, and consider Green’s function and interaction potential matrices defined as

$$
G = \begin{bmatrix} G_{1,1} & G_{1,2} \\ G_{2,1} & G_{2,2} \end{bmatrix}; \quad U = \begin{bmatrix} U_{1,1} & U_{1,2} \\ U_{2,1} & U_{2,2} \end{bmatrix}, \tag{2.12}
$$

where the off-diagonal terms representing propagation between bands are zero for the bare Green’s function matrix (i.e., an electron can only propagate between bands because of some interaction). The bare Green’s function matrix is then

$$
G^{(0)} = \begin{bmatrix} G^{(0)}_{1,1} & 0 \\ 0 & G^{(0)}_{2,2} \end{bmatrix}. \tag{2.13}
$$
Substituting the matrix Green’s function into the matrix form of Dyson’s equation, Eqn. (1.7), we have [6]

\[
G_{k\omega}^{-1} = \left( G_{k\omega}^{(0)} \right)^{-1} - \Sigma_k
= \begin{pmatrix}
\left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} & -\Sigma_{k,1,2} \\
-\Sigma_{k,2,1} & \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2}
\end{pmatrix},
\]

Taking the inverse of this matrix gives the final form of the dressed Green’s function matrix

\[
G_{k\omega} = \frac{1}{\left| G_{k\omega}^{-1} \right|} \begin{pmatrix}
\left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} & \Sigma_{k,1,2} \\
\Sigma_{k,2,1} & \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2}
\end{pmatrix},
\]

where the determinant is

\[
\left| G_{k\omega}^{-1} \right| = \left[ \left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} \right] \left[ \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2} \right] - \Sigma_{k,1,2} \Sigma_{k,2,1},
\]

and the four elements of the dressed Green’s function matrix are now given by

\[
G_{k\omega,1,1} = \left[ \left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} \right] - \frac{\Sigma_{k,1,2} \Sigma_{k,2,1}}{\left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2}},
\]

\[
G_{k\omega,2,2} = \left[ \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2} \right] - \frac{\Sigma_{k,1,2} \Sigma_{k,2,1}}{\left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1}},
\]

\[
G_{k\omega,1,2} = \left[ \left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} \right] \left[ \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2} \right] - \Sigma_{k,2,1},
\]

\[
G_{k\omega,2,1} = \left[ \left( G_{k\omega,1,1}^{(0)} \right)^{-1} - \Sigma_{k,1,1} \right] \left[ \left( G_{k\omega,2,2}^{(0)} \right)^{-1} - \Sigma_{k,2,2} \right] - \Sigma_{k,1,2}.
\]

The interband (off-diagonal) self-energy elements appear as corrections to the intraband (diagonal) Green’s function elements, \( G_{k\omega,1,1} \) and \( G_{k\omega,2,2} \). In the limit of small interband self-energy contributions, these corrections vanish, being of order \( \mathcal{O}(\Sigma_{k,1,2} \Sigma_{k,2,1}) \). Similarly, the interband elements of the Green’s function will also disappear as the interband elements of the self-energy approach zero, as interband propagation occurs only in the presence of interband self-energy contributions. Therefore, in the limit of vanishing interband self-energy elements, the dressed Green’s function matrix is diagonal (i.e. intraband only), with propagation between bands and the intraband propagation governed by the dressed single-band Green’s functions,

\[
\lim_{\Sigma_{i,j \neq i} \to 0} G_{k\omega,a,a} = G_{k\omega,a},
\]

\[
\lim_{\Sigma_{i,j \neq i} \to 0} G_{k\omega,a,b \neq a} = 0.
\]

The matrix elements Eqns. (2.16-2.19) can then be simplified by expressing each self-energy as a sum of its real and imaginary parts \((\Sigma = \Sigma' + i\Sigma'')\), and making use of the knowledge that, because the bare and interacting Green’s function matrices are
Hermitian, the self-energy matrix must also be Hermitian (giving $\Sigma_{k,\omega;1,2} = \Sigma_{k,\omega;1,2}^\dagger$):

$$G_{k,\omega;2,2} = \left[ \left( G_{k,\omega;2,2}^{(0)} \right)^{-1} - \Sigma_{k,\omega;2,2} - i \Sigma'_{k,\omega;2,2} \right]^{-1} \left( \left( G_{k,\omega;1,1}^{(0)} \right)^{-1} - \Sigma'_k - i \Sigma''_k \right). \quad (2.20)$$

We define the multi-band versions of $\eta_{k,\omega}$ and $\Gamma_{k,\omega}$ (Eqns. (2.2) and (2.3)) as

$$\eta_{k,\omega;a,a} = \omega - \varepsilon_{k,a,a} - \Sigma'_{k,\omega;a,a}, \quad \Gamma_{k,\omega;a,a} = \Sigma''_{k,\omega;a,a} - \delta,$$  

where $\varepsilon_{k,a,a}$ refers to the dispersion for the $a$ band. We find a simpler expression for the intraband Green’s function element (for $a, b \in \{1, 2\}, b \neq a$)

$$G_{k,\omega;a,a} = \left[ \eta_{k,\omega;a,a} - i \Gamma_{k,\omega;a,a} - \frac{\left| \Sigma_{k,\omega;b,a} \right|^2}{\eta_{k,\omega;b,b} - i \Gamma_{k,\omega;b,b}} \right]^{-1} \left[ \eta_{k,\omega;a,a} \left( \eta_{k,\omega;b,b} + \Gamma_{k,\omega;b,b}^2 \right) - \left| \Sigma_{k,\omega;b,a} \right|^2 \eta_{k,\omega;b,b} + i \Gamma_{k,\omega;b,b} \right]^{-1}$$

and, for the interband elements of the dressed Green’s function matrix,

$$G_{k,\omega;1,2} = \left[ \eta_{k,\omega;a,a} - i \Gamma_{k,\omega;a,a} - \frac{\left| \Sigma_{k,\omega;b,a} \right|^2}{\eta_{k,\omega;b,b} - i \Gamma_{k,\omega;b,b}} \right]^{-1} \left[ \eta_{k,\omega;a,a} \left( \eta_{k,\omega;b,b} + \Gamma_{k,\omega;b,b}^2 \right) - \left| \Sigma_{k,\omega;b,a} \right|^2 \eta_{k,\omega;b,b} + i \Gamma_{k,\omega;b,b} \right]^{-1}$$

$$\left[ \left( G_{k,\omega;b,b}^{(0)} \right)^{-1} - \Sigma_{k,\omega;b,b} - i \Sigma'_{k,\omega;b,b} \right]^{-1} \left( \left( G_{k,\omega;1,1}^{(0)} \right)^{-1} - \Sigma'_k - i \Sigma''_k \right). \quad (2.23)$$

which, as expected, is proportional to the interband self-energy, so that, if the interband self-energy contribution vanishes, so does the interband Green’s function (i.e. $\lim_{\omega \to 0} G_{a,b \neq a} = G_{a,b \neq a}^{(0)} = 0$).

2.1.4 The Spectral Density Function (Two Bands)

For the case of a two-band material, we consider first the intraband (diagonal) terms $G_{k,\omega;1,1}$ and $G_{k,\omega;2,2}$, again taking the low energy limit, before considering the interband (off-diagonal) terms $G_{k,\omega;1,2} = G_{k,\omega;2,1}^{\dagger}$ in the same manner.
Intraband Elements

For the intraband (diagonal) elements of the Green’s function matrix, Eqn. (2.23), the spectral densities are (for \(a, b \in \{1, 2\}, b \neq a\))

\[
A_{k,a,a} = -2 \left( \eta^2_{k,\omega,b} + \Gamma^2_{k,\omega,b} \right) \left[ \Gamma_{k,\omega,a,a} \left( \eta^2_{k,\omega,b} + \Gamma^2_{k,\omega,b} \right) + |\Sigma_{k,\omega,a,b}|^2 \Gamma_{k,\omega,b} \right]
\]

\[
\eta_{k,\omega,a,a} \left( \eta^2_{k,\omega,b} + \Gamma^2_{k,\omega,b} \right) - |\Sigma_{k,\omega,a,b}|^2 \eta_{k,\omega,b}^2 \right] + \left[ \Gamma_{k,\omega,a,a} \left( \eta^2_{k,\omega,b} + \Gamma^2_{k,\omega,b} \right) + |\Sigma_{k,\omega,a,b}|^2 \Gamma_{k,\omega,b} \right]^2.
\]

(2.25)

Again, we take the low energy limit, in the two band case given by \(\Gamma_{a,b} = \Sigma'^{\prime}_{a,b} \rightarrow 0\) \(\forall a, b \in \{1, 2\}\). The small \(\Gamma\) limit is equivalent to a divergence of the quasiparticle lifetime, and, as such, we equate this limit with the existence of well-defined quasiparticles. We discard terms of order \(O\left(\Sigma^{\prime 2}_{k,\omega,a,b}\right)\) and obtain

\[
A_{k,a,a} = -2 \eta^2_{k,\omega,b} \left[ \Gamma_{k,\omega,a,a} \eta^2_{k,\omega,b} + \Sigma'^{\prime 2}_{k,\omega,a,b} \Gamma_{k,\omega,b} \right]
\]

\[
\left[ \eta_{k,\omega,a,a} \eta^2_{k,\omega,b} - \Sigma'^{\prime 2}_{k,\omega,a,b} \eta_{k,\omega,b} \right]^2 + \left[ \Gamma_{k,\omega,a,a} \eta^2_{k,\omega,b} + \Sigma'^{\prime 2}_{k,\omega,a,b} \Gamma_{k,\omega,b} \right]^2.
\]

(2.26)

We can further simplify the expression by assuming that the interband self-energy \(\Sigma_{k,\omega,1,2}\) is much smaller than the single band self-energies, which gives the low-energy limits of the spectral density functions,

\[
\lim_{\Gamma \rightarrow 0} A_{k,a,a} = \lim_{\Gamma \rightarrow 0} \frac{-2 \eta^2_{k,\omega,b} \Gamma_{k,\omega,a,a}}{\eta_{k,\omega,a,a} \eta^2_{k,\omega,b} - \Sigma'^{\prime 2}_{k,\omega,a,b} \eta_{k,\omega,b}} = \frac{-2 \eta^2_{k,\omega,b} \Gamma_{k,\omega,a,a}}{\eta_{k,\omega,a,a} \eta^2_{k,\omega,b} - \Sigma'^{\prime 2}_{k,\omega,a,b} \eta_{k,\omega,b}}
\]

\[
\lim_{\Gamma \rightarrow 0} (A_{k,a,a})^2 = \frac{-2 \eta^2_{k,\omega,b} \Gamma_{k,\omega,a,a}}{\eta_{k,\omega,a,a} \eta^2_{k,\omega,b} - \Sigma'^{\prime 2}_{k,\omega,a,b} \eta_{k,\omega,b}}.
\]

(2.27)

(2.28)

It can be seen from Eqn. (2.28) that, in the limit of vanishing interband self-energy, the spectral density function for band \(a\) depends only on the properties of band \(a\) and the two bands represent independent channels.

Interband Elements

Similarly, the spectral density function for the interband (off-diagonal) elements can be expressed as

\[
A_{k,a,b} = \frac{(\Sigma_{k,a,b})^2}{\sum_{k,a,b} (\Sigma'_{k,a,b} (\Gamma_{k,a,a} \eta_{k,b} + \eta_{k,a,a} \Gamma_{k,b,a}) + \Sigma''_{k,a,b} (\eta_{k,a,a} \eta_{k,b} - \Gamma_{k,a,a} \Gamma_{k,b,a} - (\Sigma_{k,a,b})^2))}
\]

(2.29)

where we have defined

\[
Q = \left[ \Sigma'_{k,a,b} (\eta_{k,a,a} \eta_{k,b} - \Gamma_{k,a,a} \Gamma_{k,b,a} - (\Sigma_{k,a,b})^2) - \Sigma''_{k,a,b} (\Gamma_{k,a,a} \eta_{k,b} + \eta_{k,a,a} \Gamma_{k,b,a}) \right]^2 + \left[ \Sigma'_{k,a,b} (\Gamma_{k,a,a} \eta_{k,b} + \eta_{k,a,a} \Gamma_{k,b,a}) + \Sigma''_{k,a,b} (\eta_{k,a,a} \eta_{k,b} - \Gamma_{k,a,a} \Gamma_{k,b,a} - (\Sigma_{k,a,b})^2) \right]^2.
\]

(2.30)

If we now take the low energy limit once more, and again discard terms of order \(O\left(\Sigma^{\prime 2}_{k,\omega,a,b}\right)\) in both the numerator and denominator, we find the following expression,

\[
A_{k,a,b} = \frac{\Sigma_{k,a,b} (\Gamma_{k,a,a} \eta_{k,b} + \eta_{k,a,a} \Gamma_{k,b,a})}{\eta_{k,a,a} \eta_{k,b} - \Sigma'_{k,a,b}} + \frac{\Sigma'_{k,a,b}}{\eta_{k,a,a} \eta_{k,b} - \Sigma'_{k,a,b}}.
\]

(2.31)

which clearly vanishes in the limits \(\Sigma_{k,\omega,a,b} \rightarrow 0\) (no interband scattering) or \(\Sigma_{k,\omega,a,b} \rightarrow \infty\) (strong interband scattering). In any case, in the conductivity derivation below, the interband terms do not play a role, as the current-current correlation function restricts the currents to the intraband case.
2.2 Resistivity and the Kubo Formula for Conductivity

To derive the multiple band Kubo formula for conductivity, we first define the relevant interacting Hamiltonian, in terms of $c_{p,\sigma,a}^\dagger$ and $c_{p,\sigma,a}$, which respectively create and annihilate an electron with momentum $p$ and spin $\sigma$ in band $a$,

$$
H = H_0 + V,
$$

(2.32)

$$
H_0 = \sum_{p,\sigma,a} \xi_{p,\sigma,a} c_{p,\sigma,a}^\dagger c_{p,\sigma,a},
$$

(2.33)

where $V(q)$ is the interaction (scattering) potential. The electronic current density operator $j$ and the current-current correlation function $\pi(\omega)$ are given by

$$
j_\alpha = -e \sum_{p,\sigma,a} v_{p,\sigma,a} c_{p,\sigma,a}^\dagger c_{p,\sigma,a},
$$

(2.35)

$$
\pi_{\alpha\gamma}(\omega_n) = -\frac{1}{V_D} \int_0^\beta d\tau e^{i\omega_n\tau} \langle T_{\tau} j_\alpha(\tau) j_\gamma(0) \rangle,
$$

(2.36)

where $V_D$ is the $D$-dimensional volume, $-e$ is the charge on an electron, $v_{p,\sigma,a} = \frac{\partial H_0}{\partial p_{\sigma}} = \frac{1}{\hbar} \frac{\partial H_0}{\partial k_{\sigma,a}}$ is the $\alpha$-component of the (group) velocity of an electron with momentum $p = \hbar k$ and energy $\varepsilon_p$, $\tau$ is the imaginary time ($\beta = \frac{1}{k_B T}$), $T_{\tau}$ is the imaginary time ordering operator and $\langle \cdots \rangle$ denotes an expectation value over the system. The $n$th fermion Matsubara frequency, $\omega_n = \frac{i(2n+1)\pi k_B T}{\hbar}$ gives the location of the $n$th pole of the Fermi-Dirac distribution in the complex plane at zero temperature. Working in the interaction picture, the correlation function can be evaluated via an $S$-matrix expansion

$$
\pi_{\alpha\gamma}(\omega_n) = -\frac{1}{V_D} \int_0^\beta d\tau e^{i\omega_n\tau} \langle T_{\tau} S(\beta) e^{\tau H_0} j_\alpha(\tau) \rangle e^{-\tau H_0 j_\gamma(0)}
$$

(2.37)

$$
= \sum_{n=0}^\infty \pi_{\alpha\gamma}^{(n)}(\omega_n),
$$

(2.38)

where $\pi_{\alpha\gamma}^{(n)}(\omega_n)$ is the $n$-th order term of the expansion. The lowest order (non-interacting) term is given by

$$
\pi_{\alpha\gamma}^{(0)}(\omega_n) = -\frac{e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n\tau} \sum_{p,p',\sigma,\sigma',a,a'} v_{p,\sigma,a} v_{p',\sigma',a'} \langle T_{\tau} c_{p,\sigma,a}^\dagger(\tau) c_{p,\sigma,a}(\tau) c_{p',\sigma',a'}^\dagger(0) c_{p',\sigma',a'}(0) \rangle.
$$

(2.39)

We can then use Wick’s theorem to rearrange the terms in the correlation function Eqn. (2.39), to express the non-interacting correlation function in terms of non-interacting Green’s functions [6]

$$
\pi_{\alpha\gamma}^{(0)}(\omega_n) = -\frac{e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n\tau} \sum_{p,p',\sigma,\sigma',a,a'} v_{p,\sigma,a} v_{p',\sigma',a'} \langle T_{\tau} c_{p,\sigma,a}^\dagger(\tau) c_{p,\sigma,a}(\tau) c_{p',\sigma',a'}^\dagger(0) c_{p',\sigma',a'}(0) \rangle
$$

(2.40)
where the ensemble averages are only nonzero if the momenta, spin and band indices of the created and annihilated particles are equal (i.e. $p = p', \sigma = \sigma', a = a'$). Using the definition of the non-interacting Green’s functions, [5, 6]

$$\pi_{\alpha\gamma}^{(0)}(i\omega_n) = \frac{\beta}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \sum_{p,\sigma,a} v_{p,\sigma,a} v_{p,\gamma,a} \langle T_\tau c_{p,\sigma,a}^\dagger(0) c_{p,\sigma,a}(0) \rangle$$

$$= \frac{2\beta}{V_D} \sum_p \sum_{\sigma,a} v_{p,\sigma,a} v_{p,\gamma,a} \int_0^\beta d\tau e^{i\omega_n \tau} G_{a,a}^{(0)}(p;\tau) G_{a,a}^{(0)}(p;\tau),$$

(2.41)

where the sum over spin states has been performed to give the factor of 2. The correlation function Eqn. (2.41) involves only non-interacting Green’s functions and, as such, involves no mechanism for relaxation. Thus, the resistivity from Eqn. (2.41) will vanish. We can insert interactions into the non-interacting correlation function by replacing the bare Green’s functions with their corresponding dressed form, where the interactions are taken into account by the self-energy.

The factor $\int_0^\beta d\tau e^{i\omega_n \tau} G_{a,a}(p;\tau) G_{a,a}(p;\tau)$ is simply the Fourier transform of the convolution of two Green’s functions in the Matsubara formalism, which can be evaluated to give the correlation function, in terms of Matsubara Green’s functions (which, after analytic continuation, give the finite temperature Green’s functions) [6],

$$\pi_{\alpha\gamma}(i\omega_n) = \frac{2\beta}{V_D} \sum_p \sum_{\sigma,a} v_{p,\sigma,a} v_{p,\gamma,a} \int_0^\beta d\tau e^{i\omega_n \tau} G_{a,a}(p;\tau) G_{a,a}(p;\tau)$$

$$= \frac{2\beta}{V_D} \sum_p \sum_{\sigma,a} v_{p,\sigma,a} v_{p,\gamma,a} \frac{1}{\beta} \sum_{ip} G_{a,a}(p;ip + i\omega) G_{a,a}(p;ip).$$

(2.42)

The sum over Matsubara frequencies is performed by moving to the spectral representation, where the interacting Green’s functions are given by [5, 6]

$$G_{a,a}(p; i\omega) = \int \frac{d\varepsilon}{2\pi} A_{a,a}(p, \varepsilon) \frac{1}{ih\omega - \varepsilon},$$

(2.43)

and the summation $S_{a,a}(i\omega_n) = \sum_{ip} G_{a,a}(p; ip + i\omega) G_{a,a}(p; ip)$ is given by

$$S_{a,a}(i\omega_n) = \frac{1}{\beta} \sum_{ip} G_{a,a}(p; ip + i\omega) G_{a,a}(p; ip)$$

$$= \int \frac{d\varepsilon_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A_{a,a}(p, \varepsilon_2) \frac{1}{\beta} \sum_{ipm} \frac{1}{ih\omega_m + i\varepsilon_1} \frac{1}{ih\omega_m - \varepsilon_2}$$

(2.44)

$$= \int \frac{d\varepsilon_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A_{a,a}(p, \varepsilon_2) S_0(i\omega_n),$$

(2.45)

where $S_{0,a,a}(i\omega_n) \equiv \frac{1}{\beta} \sum_{ip} G_{a,a}^{(0)}(p; ip + i\omega) G_{a,a}^{(0)}(p; ip) = \frac{n_\uparrow(\varepsilon_2) - n_\uparrow(\varepsilon_1)}{ih\omega_n + \varepsilon_2 - \varepsilon_1}$ is computed via a contour integral. First defining the function

$$f(z) = \frac{1}{hz + ih\omega_n - \varepsilon_1} \frac{1}{hz - \varepsilon_2}$$

(2.46)

we wish to find the sum of $f(z)$ at $z = ip_n$, the Matsubara frequencies, which are just the locations of the poles of the Fermi-Dirac distribution. By performing a contour integral over $f(z)n_f(z)$ and choosing the contour such that the integral vanishes, we can
equate the summation with the residues of \( f(z) \),

\[
I = \lim_{R \to \infty} \int \frac{dz}{2\pi i} f(z)n_f(z) = \lim_{R \to \infty} \int \frac{dz}{2\pi i} \frac{1}{h\omega_n - \varepsilon_1 + \frac{1}{h\varepsilon_2 - \varepsilon_1}n_f(z)} 0 = \sum_i r_i n_f(z_i) + \sum_{ip_m} f(ip_m),
\]

\[
S_{0,a,a}(i\omega_n) = \sum_{ip_m} f(ip_m) = -\sum_i r_i n_f(z_i) = \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{ih\omega_n + \varepsilon_2 - \varepsilon_1}.
\]

Thus, the expression for \( S_{a,a}(i\omega_n) \) becomes

\[
S_{a,a}(i\omega_n) = \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int dz_2 A_{a,a}(p, \varepsilon_2) \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{h\omega + i\varepsilon_2 - \varepsilon_1}.
\]

Performing the analytic continuation, \( i\omega_n = \omega + i\delta \), we obtain the retarded value,

\[
S_{a,a}(\omega) = \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int dz_2 A_{a,a}(p, \varepsilon_2) \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{h\omega + i\varepsilon_2 - \varepsilon_1},
\]

\[
\text{Im} \{ S_{a,a}(\omega) \} = \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int dz_2 A_{a,a}(p, \varepsilon_2) -\pi(n_f(\varepsilon_2) - n_f(\varepsilon_1)) \delta (h\omega + \varepsilon_2 - \varepsilon_1).
\]

Taking the limit \( \delta \to 0 \) results in the creation of a Dirac delta function \( \delta(f(\omega)) \approx \lim_{\eta \to 0} \eta \delta(\omega) \) in the integral,

\[
\lim_{\delta \to 0} \text{Im} \{ S_{a,a}(\omega) \} = -\pi \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) \int dz_2 A_{a,a}(p, \varepsilon_2) (n_f(\varepsilon_2) - n_f(\varepsilon_1)) \delta (h\omega + \varepsilon_2 - \varepsilon_1)
\]

\[
= -\int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) A_{a,a}(p, \varepsilon_2 + \omega) (n_f(\varepsilon_2) - n_f(\varepsilon_2 + h\omega)),
\]

so, the current-current correlation function is given by

\[
\text{Im} \{ \pi_{\alpha\gamma}(\omega) \}_R = -\frac{e^2}{V_D} \sum_p \sum_a v_p^{\alpha,a} v_p^{\gamma,a} \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) A_{a,a}(p, \varepsilon_2 + \omega) (n_f(\varepsilon_2) - n_f(\varepsilon_2 + h\omega)).
\]

The conductivity is then found by taking the zero frequency limit of the retarded current-current correlation function divided by the frequency \( \omega \),

\[
\sigma_{\alpha\gamma} = \lim_{\omega \to 0} \frac{e^2}{V_D} \sum_p \sum_a v_p^{\alpha,a} v_p^{\gamma,a} \int \frac{dz_1}{2\pi} A_{a,a}(p, \varepsilon_1) A_{a,a}(p, \varepsilon_2 + \omega) \frac{h(n_f(\varepsilon_2) - n_f(\varepsilon_2 + h\omega))}{h\omega}
\]

\[
= e^2 h \sum_a \int_{-\infty}^{\infty} \frac{d^Dp}{(2\pi h)^D} v_p^{\alpha,a} v_p^{\gamma,a} \int_{-\infty}^{\infty} d\varepsilon \frac{A_{a,a}^2(p, \varepsilon)}{\frac{d\eta}{d\varepsilon}} \left( \frac{dn_f(\varepsilon)}{d\varepsilon} \right).
\]

In three dimensions, the conductivity is given by

\[
\sigma_{\alpha\gamma} = e^2 h \sum_a \int_{-\infty}^{\infty} \frac{d^3p}{(2\pi h)^3} v_p^{\alpha,a} v_p^{\gamma,a} \int_{-\infty}^{\infty} d\varepsilon \frac{A_{a,a}^2(p, \varepsilon)}{\frac{d\eta}{d\varepsilon}} \left( \frac{dn_f(\varepsilon)}{d\varepsilon} \right).
\]

2.2.1 Expression in terms of the Self-Energy

Using the previously derived expressions for the low energy limit of the diagonal spectral density function elements, with minimal interband scattering \( \Sigma_{k,\omega_{1,2}} \ll \Sigma_{k,\omega_{\alpha\beta}} \), Eqn. (2.28), we arrive at the definition of a diagonal component of the conductivity
For the case where the density of states and average velocity squared in each band are equal, the conductivity is given by

\[ \sigma_{xx} = e^2 \hbar \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} \left( -\frac{2\pi \delta (\varepsilon_{k,\omega,1})}{\Gamma_{k,\omega,1}} v_{k,x,1}^2 + \frac{2\pi \delta (\varepsilon_{k,\omega,2})}{\Gamma_{k,\omega,2}} v_{k,x,2}^2 \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) . \]

Defining the average squared x-component of the group velocity for band \( a \) as \( \langle v_{k,x,a}^2 \rangle \), and assuming that \( v_{k,x,a}^2 \) varies slowly in the direction perpendicular to the Fermi surface, we use the sharply peaked nature of the derivative of the Fermi-Dirac distribution to find the more compact definition of the two band conductivity,

\[ \sigma_{xx} = \sum_{a=1}^{2} \frac{e^2 \hbar \langle v_{k,x,a}^2 \rangle}{2} \int_{-\infty}^{\infty} \frac{d^3k}{(4\pi^3)} Z_{a,a} \delta (Z_{a,a} \varepsilon_F - Z_{a,a} \varepsilon_{k,\omega,0,a}) \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma_{k,\omega,0,a}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) , \quad (2.53) \]

which is simply the sum in series of the two individual bands’ conductivities,

\[ \sigma_{xx} = \sum_{a=1}^{2} \frac{e^2 \hbar \langle v_{k,x,a}^2 \rangle}{2} \left( D_0 (\varepsilon_F) \right)_a \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma_{k,\omega,0,a}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) , \quad (2.54) \]

where, in the first line of Eqn. (2.54) we have defined the density of states for band \( i \), \( (D_0 (\varepsilon))_i = \int_{-\infty}^{\infty} \frac{d^3k}{(4\pi^3)} [\delta (\varepsilon_{k,i} - \varepsilon_F)] \) and in the last line, we have defined the conductivity of individual bands \( \sigma_{xx,i}^{(0)} \).

For the case where the density of states and average velocity squared in each band are equal, the conductivity is given by

\[ \sigma_{xx}^{(0)} = \frac{e^2 \hbar \langle v_{k,x,a}^2 \rangle}{2m^2} \left( D_0 (\varepsilon_F) \right) \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma_{k,\omega,1,1}} + \frac{1}{\Sigma_{k,\omega,2,2}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) , \quad (2.55) \]

It is clear that Eqn. (2.55) has a form similar to that of the one band case (see Eqn. (A.21), Appendix A.1), with the two imaginary self-energies adding in parallel. It immediately follows that the resistivities of the two bands must add in parallel, recovering Matthiessen’s rule [3].

### 2.2.2 The Quadratic Resistivity Coefficient

For a Fermi liquid at low temperatures, the resistivity is known to be related to the temperature by Eqn. (1.1),

\[ \rho = \rho_0 + AT^2 , \quad (2.56) \]
\[ A = \frac{1}{T^2} \left( \left[ \sigma_{xx}^{(0)} (T) \right]^{-1} - \left[ \sigma_{xx}^{(0)} (T = 0) \right]^{-1} \right) . \quad (2.57) \]

For determining the conductivity, we make use of a generalised form of the phenomenological model for the imaginary part of the self energy proposed by Miyake, Matsuura and Varma (MMV) [34]. To determine the quadratic resistivity coefficient in the two band case, we assume that the individual band self-energies follow the same energy dependence as outlined by MMV,

\[ \Sigma_{k,\omega,0,a} = -\frac{\hbar}{2\tau_{0,a}} - s_a \frac{\varepsilon^2 + (\pi k_b T)^2}{\varepsilon_{0,a}^2} \quad \text{for} \quad |\varepsilon^2 + (\pi k_b T)^2| < \varepsilon_{0,a}^2 , \]
\[ = -\left( \frac{\hbar}{2\tau_{0,a}} + s_a \right) F \left( \frac{\varepsilon^2 + (\pi k_b T)^2}{\varepsilon_{0,a}^2} \right) \quad \text{for} \quad |\varepsilon^2 + (\pi k_b T)^2| > \varepsilon_{0,a}^2 , \quad (2.58) \]
where the energy $\varepsilon$ is measured from the Fermi level, $\tau_0^{-1}$ is the impurity scattering rate, $2s_a/\hbar$ is the electron-electron scattering rate, $F(x)$ is a monotonically decreasing function with $F(1) = 1$ and $F(\infty) = 0$ and $\varepsilon_{0,a}$ is an energy scale characterising the strength of the many-body correlations ($\varepsilon_{0,a} \approx Z_a\varepsilon_F$, with $Z_a$ the mass renormalisation factor in band $a$).

In the pure limit the constant term in the resistivity, which arises solely due to quasiparticle-impurity scattering, vanishes. Since the quasiparticle-quasiparticle contribution is proportional to the energy measured from the Fermi energy, it too vanishes at zero temperature, when all quasiparticles are restricted to the Fermi surface. As such, the constant term in the resistivity also vanishes, and the finite temperature imaginary self-energy and conductivity are given by

$$\frac{1}{\Sigma_{k,c,a,a}^{\nu}} = - \frac{\varepsilon_{0,a}^2}{s_{p,a}} \left( \varepsilon^2 + (\pi k_b T)^2 \right),$$

$$\sigma_{xx}^{(0)} = \frac{e^2}{2} \left( \frac{\varepsilon^2}{s_{p,1}} \left( \varepsilon^2 + (\pi k_b T)^2 \right) \right) \left( - \frac{dn_f(\varepsilon)}{d\varepsilon} \right)$$

$$+ \frac{e^2}{2} \left( \frac{\varepsilon_{0,2}^2}{s_{p,2}} \left( \varepsilon^2 + (\pi k_b T)^2 \right) \right) \left( - \frac{dn_f(\varepsilon)}{d\varepsilon} \right),$$

where $s_a$ in the pure limit is given by the unitary limit of scattering, $s_{p,a} = \frac{2s_a}{\pi \hbar F_0(\varepsilon_F)} [20, 34]$. The derivative in Eqn. (2.60) is easily evaluated and simplified via a change of variables $x = \frac{\varepsilon - \mu}{k_b T}$

$$\frac{dn_f(\varepsilon, T)}{d\varepsilon} = - \frac{1}{k_b T} \left( \frac{e^{\varepsilon - \mu}}{e^{\varepsilon - \mu} + 1} \right)^{-2} e^{\varepsilon - \mu}$$

$$= - \frac{1}{k_b T} \frac{e^x}{(e^x + 1)^2}$$

$$= - \frac{1}{4k_b T} \frac{1}{e^{x/2} + e^{-x/2}}$$

$$= - \frac{1}{4k_b T} \text{sech}^2 \left( \frac{x}{2} \right),$$

$$\frac{1}{\Sigma_{k,c,a,a}^{\nu}} = - \frac{x_{0,a}^2}{s_{p,a}} \left( x^2 + \pi^2 \right),$$

Each of the energy integrals can then be evaluated (see Appendix A.3.1) to give $\int_{-\infty}^{\infty} dx \text{sech}^2 \left( \frac{x}{2} \right) = \frac{1}{4}$, and will contribute a factor of

$$\frac{e_{0,a}^2}{12k_b^2 T^2 s_{p,a}} = \frac{e_{0,a}^2(D_0(\varepsilon_F))_a}{8k_b^2 T^2 s_{p,a}}.$$ 

The two-band $A$ coefficient then has the form

$$A = \left( \frac{e^2}{24k_b^2} \frac{\varepsilon_{0,1}^2}{s_{p,1}} \left( D_0(\varepsilon_F) \right)_1 \right)^{-1} + \left( \frac{e^2}{24k_b^2} \frac{\varepsilon_{0,2}^2}{s_{p,2}} \left( D_0(\varepsilon_F) \right)_2 \right)^{-1}$$

$$= \left( \frac{\pi e^2}{16k_b^2} \frac{\varepsilon_{0,1}^2}{n_1} \left( D_0(\varepsilon_F) \right)_1 \right)^{-1} + \left( \frac{\pi e^2}{16k_b^2} \frac{\varepsilon_{0,2}^2}{n_2} \left( D_0(\varepsilon_F) \right)_2 \right)^{-1}$$

$$= \left( \frac{16k_b^2}{\pi e^2} \left( \frac{\varepsilon_{0,1}^2}{n_1} \right) \left( D_0(\varepsilon_F) \right)_1 \right)^{-1} + \left( \frac{16k_b^2}{\pi e^2} \left( \frac{\varepsilon_{0,2}^2}{n_2} \right) \left( D_0(\varepsilon_F) \right)_2 \right)^{-1}$$

$$= \left( A_1^{-1} + A_2^{-1} \right)^{-1},$$

where $A_1$ and $A_2$ are the one-band coefficients due to each band (see Appendix A.1 for the derivation of the Kadowaki-Woods ratio in one-band materials).
2.3 Heat Capacity

The self-energy, being causal in the time domain, satisfies the conditions for the Kramers-Kronig relations in the frequency domain. Knowledge of the form of the imaginary part of the self-energy is then sufficient to determine the real part, which appears in the definition of the renormalisation factor and therefore in the expression for the heat capacity. The real part of the self-energy within a single band is then

\[
\Sigma'(\varepsilon) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\varepsilon' \frac{\Sigma''(\varepsilon')}{\varepsilon' - \varepsilon}
\]

\[
= -\frac{1}{\pi} P \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon' \left( \frac{\hbar}{2\tau_0} + s \frac{\varepsilon'^2 + (\pi k_b T)^2}{\varepsilon_0^2} \right) \frac{1}{\varepsilon' - \varepsilon} - \frac{1}{\pi} P \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon' \left( \frac{\varepsilon'^2 + (\pi k_b T)^2}{\varepsilon_0^2} \right)^{1/2} \frac{1}{\varepsilon' - \varepsilon}.
\]

In the low temperature, low impurity limit, the real part of the self-energy becomes

\[
\lim_{T \to 0} \lim_{\tau_0 \to \infty} \Sigma'(\varepsilon) = -\frac{s_P}{\pi \varepsilon_0} P \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon' \frac{\varepsilon'^2}{\varepsilon' - \varepsilon}
\]

\[
= -s_p \int_{-\infty}^{\varepsilon_0} d\varepsilon' \frac{\varepsilon'}{\varepsilon_0} \left( \frac{1}{\varepsilon' - \varepsilon} \right) - s_p \int_{\varepsilon_0}^{\infty} d\varepsilon' \frac{\varepsilon'}{\varepsilon_0} \left( \frac{1}{\varepsilon' - \varepsilon} \right).
\]

where we have first assumed that the pole of the integral, \(\varepsilon' = \varepsilon\), occurs within the range \(|\varepsilon'| \leq |\varepsilon_0|\), and then taken the pure (low impurity), low temperature limit. The first integral on the right hand side of Eqn. (2.64) can be evaluated using the definition
of the Cauchy principle value, and introducing a change of variables \((x = \varepsilon' - \varepsilon)\) that shifts the pole \((\varepsilon' = \varepsilon)\) to the origin,

\[
\frac{s_p}{\pi \varepsilon_0^2} P \int_{-\varepsilon_0}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon' - \varepsilon} = \frac{s_p}{\pi \varepsilon_0^2} \lim_{\delta \to 0} \left[ \int_{-\varepsilon_0}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon' - \varepsilon} + \int_{\varepsilon + \delta}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon' - \varepsilon} \right]
\]

\[
= \frac{s_p}{\pi \varepsilon_0^2} \lim_{\delta \to 0} \left[ \int_{\delta}^{\varepsilon_0 - \varepsilon} \frac{\left[ \varepsilon_0 - \varepsilon \right]}{\varepsilon' - \varepsilon} d\varepsilon' + \int_{\varepsilon + \delta}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon' - \varepsilon} \right]
\]

\[
= \frac{s_p}{\pi \varepsilon_0^2} \lim_{\delta \to 0} \left( \left[ \varepsilon_0 - \varepsilon \right] + \left[ \varepsilon_0 - \varepsilon \right] \right) - \left[ \varepsilon_0 - \varepsilon \right] \right)
\]

\[
= \frac{s_p}{\pi \varepsilon_0^2} \left( \frac{\varepsilon_0}{\varepsilon_0 + \varepsilon} \right)
\]

\[
= \frac{s_p}{\pi \varepsilon_0^2} \left[ \frac{2 \varepsilon_0 + \varepsilon^2 \ln \left( \frac{\varepsilon_0 - \varepsilon}{\varepsilon_0 + \varepsilon} \right) \right]
\]

\[
= \frac{s_p}{\pi} \left[ \frac{\varepsilon_0}{\varepsilon_0^2} - \left( \frac{\varepsilon_0}{\varepsilon_0} \right)^3 \right].
\]

In the last line of Eqn. (2.65) we have expanded the natural logarithm in a Taylor series and discarded terms of order \(O \left( \left( \frac{\varepsilon_0}{\varepsilon_0} \right)^5 \right)\) and higher. The remaining integrals in Eqn. (2.64) can also be evaluated by first using a change of variable \((y = \frac{\varepsilon}{\varepsilon_0}\) and \(y' = \frac{\varepsilon'}{\varepsilon_0}\) and exploiting the symmetric nature of the function \(F(y)\) about \(y = 0\),

\[
\frac{s_p}{\pi} \int_{-\infty}^{\varepsilon_0} \frac{d\varepsilon'}{\varepsilon_0} \left[ \varepsilon_0 \right] \frac{1}{\varepsilon'} - \varepsilon + \int_{\varepsilon_0}^{\infty} \frac{d\varepsilon'}{\varepsilon_0} \left[ \varepsilon_0 \right] \frac{1}{\varepsilon'} - \varepsilon
\]

\[
= \frac{s_p}{\pi} \left( \int_{-\infty}^{\infty} \frac{d\varepsilon'}{y'} \left( \frac{1}{y'} - 1 \right) + \int_{1}^{\infty} \frac{d\varepsilon'}{y'} \left( \frac{1}{y'} - 1 \right) \right)
\]

\[
= -\frac{s_p}{\pi} \left( \int_{-\infty}^{\infty} \frac{d\varepsilon'}{y'} \left( \frac{1}{y'} - 1 \right) + \int_{1}^{\infty} \frac{d\varepsilon'}{y'} \left( \frac{1}{y'} - 1 \right) \right)
\]

\[
= \frac{s_p}{\pi} \left( \frac{1}{y'} \right) \left( 1 + \frac{y}{y'} + \mathcal{O} \left( \left( \frac{y}{y'} \right)^2 \right) \right)
\]

\[
= \frac{s_p}{\pi} \left( \frac{1}{y'} \right) \left( 1 + \frac{y}{y'} + \mathcal{O} \left( \left( \frac{y}{y'} \right)^2 \right) \right)
\]

\[
= \frac{s_p}{\pi} \left( \frac{1}{y'} \right) \left( 1 - \frac{y}{y'} + \mathcal{O} \left( \left( \frac{y}{y'} \right)^2 \right) \right)
\]

\[
= \frac{2s_p}{\pi} \frac{\varepsilon}{\varepsilon_0} \xi,
\]
where $\xi$ is defined as the integral,

$$\xi = \int_1^\infty \frac{dy' F[y']}{y'^2} \sum_{n=1}^{\infty} \frac{y'^2(n-1)}{y'^2n}$$

which can be approximated by the lowest order terms in the summation, as the higher order terms will always be smaller, given that we have already assumed $|\epsilon| < |\epsilon_0|$. So, the lowest order terms will dominate the series and we have the approximation,

$$\xi \approx \int_1^\infty \frac{dy' F[y']}{y'^2}. \quad (2.68)$$

The behaviour of $\xi$ can then be analysed without the need to know the exact form of the function $F[y']$. Since $F[y']$ is a monotonically decreasing function with the conditions $F[y' = 1] = 1$ and $F[y' = \infty] = 0$, the minimum value of $\xi$ can be found by setting $F[y'] = 0$, $\forall y'$ and the maximum value by setting $F[y'] = 1$, $\forall y'$, which results in a minimum value of $\xi = 0$ and a maximum value of $\xi = 1$.

We now have an expression for the real part of the self-energy, keeping only the linear term in the first integral Eqn. (2.65), as the value of $\frac{|\epsilon|}{\epsilon_0}$ is always less than one, so the higher order terms will be negligible. Restoring band indices, the real part of the (intraband) self energy for band $a$ is

$$\Sigma'_{k,\epsilon,a,a} = -\frac{2s_{p,a}\pi}{\pi\epsilon_0,a} (1 + \xi). \quad (2.69)$$

The heat capacity is defined as the rate of change (at constant volume or pressure) of the total internal energy, $U$ of a system with respect to temperature, $T$,

$$C = \frac{dU}{dT}, \quad (2.70)$$

which is dominated at low temperatures by the electronic contribution. The internal energy in Eqn. (2.70) can be expressed as a sum of the two bands’ internal energies,

$$U = U_1 + U_2, \quad (2.71)$$

so the heat capacity becomes the sum of the heat capacity in each band

$$C = \frac{d}{dT} (U_1 + U_2) = C_1 + C_2. \quad (2.72)$$

This result agrees with our expectations, as the presence of extra bands at the Fermi energy means that extra particles are available to carry the heat energy in the system. Additionally, the quasiparticles of each of the bands could be considered an independent mechanism for energy to diffuse through the system, and, just as at higher temperatures the heat capacity is the sum of the electron and phonon contributions [3], we expect the same for the two independent bands’ contributions at low temperatures. The total heat capacity for the two band case can then be found as the sum of the individual bands’ heat capacities, each of which depends on the renormalisation factor $Z_{a} = Z_{a,a}$ of the band. If we assume that the imaginary part of each self-energy varies with energy according to Eqn. (2.58), then the real part of each self-energy has a form similar to that of Eqn. (2.69), and the two band heat capacity becomes, for an arbitrary band structure,

$$\frac{C_{el;2band}(T)}{T} = \gamma$$

$$= \frac{\pi^2 k_B^2}{3} \left[ \frac{(D_0(\epsilon_F))_1}{Z_1} + \frac{(D_0(\epsilon_F))_2}{Z_2} \right]$$

$$= \frac{\pi^2 k_B^2}{3} \left[ (D_0(\epsilon_F))_1 \left( 1 - \frac{\partial \Sigma'_{k,1,1}}{\partial \epsilon} \right) + (D_0(\epsilon_F))_2 \left( 1 - \frac{\partial \Sigma'_{k,2,2}}{\partial \epsilon} \right) \right]. \quad (2.73)$$
Inserting the appropriate expressions for the real self-energies we obtain

$$\gamma = \frac{\pi^2 k_b^2}{3} \left[ (D_0(\varepsilon_F))_1 \left( 1 + \frac{2s_{p,1}}{\varepsilon_{0,1}} (1 + \xi) \right) + (D_0(\varepsilon_F))_2 \left( 1 + \frac{2s_{p,2}}{\varepsilon_{0,2}} (1 + \xi) \right) \right],$$

and if we assume the $\frac{2s_{p,a}}{\varepsilon_{0,a}} (1 + \xi)$ terms are considerably larger than one, equivalent to assuming that the renormalised mass is greater than the bare mass (and also equivalent to the strong scattering limit, where the scattering energy $s$ is large), we arrive at a final expression for the two band $\gamma$ factor,

$$\gamma = \frac{2\pi k_b^2}{3} \left( 1 + \xi \right) \left[ \frac{s_{p,1}}{\varepsilon_{0,1}} + \frac{s_{p,2}}{\varepsilon_{0,2}} \right],$$

where the two individual bands’ $\gamma$ factors add in series, as expected [40], and, if we then insert the values for $s_{p,a} = \frac{2\pi a}{\delta(\varepsilon_F)_a}$, we obtain the expression,

$$\gamma = \frac{4k_b^2}{9} \left( 1 + \xi \right) \left[ \frac{n_1}{\varepsilon_{0,1}} + \frac{n_2}{\varepsilon_{0,2}} \right], \quad \text{(2.74)}$$

### 2.4 The Kadowaki-Woods Ratio

The Kadowaki-Woods ratio, defined as the ratio of the quadratic resistivity coefficient $A$ and the square of the linear specific heat coefficient $\gamma$, is easily calculated now that we know the form of $A$ and $\gamma$ for the two band system, Eqns. (2.63) and (2.74),

$$A = \frac{16k_b^4}{\pi e^2 \hbar} \left( \langle v_{0x,1}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,1}^2 \varepsilon_{0,1}^2 \right) + \langle v_{0x,2}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,2}^2 \varepsilon_{0,2}^2 \right) \sum_{a=1}^{2} \frac{\langle v_{0x,a}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,a}^2 \varepsilon_{0,a}^2 \rangle}{n_a},$$

$$\gamma = \frac{4k_b^2}{9} \left( 1 + \xi \right) \left[ \frac{n_1}{\varepsilon_{0,1}} + \frac{n_2}{\varepsilon_{0,2}} \right].$$

The two band Kadowaki-Woods ratio becomes

$$R_{KW:2} = \frac{16k_b^4}{\pi e^2 \hbar} \left( \langle v_{0x,1}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,1}^2 \varepsilon_{0,1}^2 \right) + \langle v_{0x,2}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,2}^2 \varepsilon_{0,2}^2 \right) \sum_{a=1}^{2} \frac{\langle v_{0x,a}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,a}^2 \varepsilon_{0,a}^2 \rangle}{n_a},$$

and if we set $\xi \approx 1$, the maximum value possible, we obtain

$$R_{KW:2} = \frac{81}{4\pi e^2 \hbar k_b^2} \left( \langle v_{0x,1}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,1}^2 \varepsilon_{0,1}^2 \right) + \langle v_{0x,2}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,2}^2 \varepsilon_{0,2}^2 \right) \sum_{a=1}^{2} \frac{\langle v_{0x,a}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,a}^2 \varepsilon_{0,a}^2 \rangle}{n_a}, \quad \text{(2.75)}$$

$$\frac{A}{\gamma^2 f_{dx:2}}(n) = \frac{81}{4\pi e^2 \hbar k_b^2}. \quad \text{(2.76)}$$

The material-independent ratio [20] for a two band material is

$$f_{dx:2}(n) = \left( \frac{n_1}{\varepsilon_{0,1}} + \frac{n_2}{\varepsilon_{0,2}} \right)^2 \left( \langle v_{0x,1}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,1}^2 \varepsilon_{0,1}^2 \right) + \langle v_{0x,2}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,2}^2 \varepsilon_{0,2}^2 \right) \sum_{b=1}^{2} \frac{\langle v_{0x,b}^2 \rangle (D_0(\varepsilon_F))^2 \varepsilon_{0,b}^2 \varepsilon_{0,b}^2 \rangle}{n_b}, \quad \text{(2.77)}$$

For comparison, the material dependent function for a one-band material, as calculated by Jacko, Fjærøst and Powell is [20]

$$f_{dx:1}(n) = n\langle v_{0x}^2 \rangle (D_0(\varepsilon_F))^2, \quad \text{(2.78)}$$

where the renormalisation, characterised by $\varepsilon_0$ cancels. It is clear from Eqn. (2.77) that, once the presence of multiple bands is taken into account, the renormalisation of $A$ and $\gamma^2$ no longer cancel each other in the Kadowaki-Woods ratio, as they do in
the one-band case, Eqn. (2.78). The renormalisation in the multi-band case will only cancel when it is independent of the band index (i.e. if \( \varepsilon_{0,i} = \varepsilon_{0,j}, \forall i, j \)), in which case we find

\[
 f_{dx:2}(n) = \left[ \sum_{a=1}^{2} n_a \right]^2 \left( \sum_{b=1}^{2} \left\langle v_{0x:b}^2 \right\rangle_b \left( \frac{D_0(\varepsilon_F)}{n_b} \right)^2 \right). \tag{2.79}
\]

**Special Cases**

In all of the following cases, the renormalisation factors are assumed to be equal for all bands, so that the renormalisation of the Kadowaki-Woods ratio is cancelled, and the material-specific function has the form of Eqn. (2.79). If the carrier densities in each band are equal \((n_1 = n_2 = \frac{2}{1})\)

\[
 f_{dx:2}(n) = 2 \left( \left\langle v_{0x:1}^2 \right\rangle_1 (D_0(\varepsilon_F))^2 \right)\frac{1}{(D_0(\varepsilon_F))^2} \\
 R_{KW:2} = \frac{81}{8\pi e^2 h k^2_0 n} \left[ \left\langle v_{0x:1}^2 \right\rangle_1 + \left\langle v_{0x:2}^2 \right\rangle_2 \right] D_0(\varepsilon_F)^2 \\
\]

alternatively, if the densities of states in each band are equal \((\left\langle D_0(\varepsilon_F) \right\rangle_1 = \left\langle D_0(\varepsilon_F) \right\rangle_2 = D_0(\varepsilon_F))\),

\[
 f_{dx:2}(n) = \frac{|n_1 + n_2|^3 \left( \left\langle v_{0x:1}^2 \right\rangle_1 + \left\langle v_{0x:2}^2 \right\rangle_2 \right) D_0(\varepsilon_F)^2}{2n_1 n_2} \\
 R_{KW:2} = \frac{81}{2\pi e^2 h k^2_0 \left[ \left\langle v_{0x:1}^2 \right\rangle_1 + \left\langle v_{0x:2}^2 \right\rangle_2 \right] D_0(\varepsilon_F)^2} \frac{n_1 n_2}{[n_1 + n_2]^3} \\n\]

and, if the carrier density \(n\), the bare average velocity at the Fermi level \(\left\langle v_F^2 \right\rangle\) and density of states \(D_0(\varepsilon_F)\) are equal for both bands,

\[
 f_{dx:2}(n) = 4 \left\langle v_{0x}^2 \right\rangle n D_0(\varepsilon_F)^2 = 4 f_{dx:1}(n) \\
 R_{KW:2} = \frac{81}{16\pi e^2 h k^2_0 \left\langle v_{0x}^2 \right\rangle n D_0(\varepsilon_F)^2} = \frac{1}{4} R_{KW:1}. \tag{2.82}
\]

**2.4.1 Extension to systems of more than two bands**

We now seek to generalise the above expression for the Kadowaki-Woods ratio in a two band material to the general many band case. This is done by generalising the \(2 \times 2\) matrix form of the self-energy and propagators defined previously to an \(N_b \times N_b\) matrix, and again neglecting the interband terms (as shown in Appendix A.2, interband contributions in the self-energy of strengths comparable to the intraband contributions lead to a vanishing conductivity).

**Conductivity, Resistivity and Heat Capacity**

The conductivity, resistivity and heat capacity can be easily extended to more than two bands, in the limit of negligible interband scattering. The many band conductivity becomes

\[
\sigma_{xx}^{(0)} = \sum_{a}^{N_b} e^2 h \left\langle v_{0x:a}^2 \right\rangle (D_0(\varepsilon_F))_a \int_{-\infty}^{\infty} d\varepsilon \left( \frac{-1}{\Sigma_{k,a,a}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) \\
= \sum_{a}^{N_b} \sigma_{xx,a}^{(0)}, \tag{2.83}
\]

with the resistivity given by the inverse. The quadratic coefficient \(A\) is then given by

\[
 A = \frac{16 k^2_0}{\pi e^2 h} \left( \sum_{a=1}^{N_b} \left\langle v_{0x:a}^2 \right\rangle (D_0(\varepsilon_F))^2 \frac{2}{n_a} \varepsilon_{0,a}^2 \right)^{-1}.
\]
while the linear heat capacity coefficient, $\gamma$ becomes

$$
C_{el,N_b \text{bands}}(T) = \gamma \frac{\pi^2 k_B^2}{3} \sum_a N_a \left( \frac{(D_0(\varepsilon_F))_a}{Z_{a}} \right)
= \frac{4k_B^2 (1 + \xi)}{9} \left[ \sum_a \frac{n_a}{\varepsilon_{0,a}} \right]. \tag{2.85}
$$

The conductivity and heat capacity, as has already been seen, are merely the sum in series of the values for individual bands, while the resistivity, being the inverse of the conductivity, is the sum in parallel of the various bands’ resistivities.

The Kadowaki-Woods Ratio

The Kadowaki-Woods ratio in the presence of more than two bands can be easily determined, with the material-specific factors in the resistivity adding in parallel and those in the heat capacity the carrier density, $n$, adding in series, so that the material-specific function $f_{dx}$ becomes

$$
f_{dx;N_b}(n) = \left( \sum_i n_i \varepsilon_{0,i} \right)^2 \left( \sum_j \frac{\langle \varepsilon_{0x;j}^2 \rangle (D_0(\varepsilon_F))^2}{n} \varepsilon_{0,j}^2 \right), \tag{2.86}
$$

with $N_b$ the number of bands in the system, which, in the limit $N_b = 1$ recovers the one band formula, Eqn. (2.78). With this choice of material dependent function, the universal Kadowaki-Woods ratio [20] has the same value as given by Eqn. (2.76). In the special case that the values for carrier density, mean velocity at the Fermi energy squared and density of states are uniform for all bands ($n_i = \frac{N_b}{N^2}$, $\langle \varepsilon_{0x;j}^2 \rangle = \langle \varepsilon_{0x}^2 \rangle$ and $(D_0(\varepsilon_F))_k = D_0(\varepsilon_F)$, $\forall i, j, k$), we arrive at

$$
f_{dx;N_b}(n) = \langle \varepsilon_{0x}^2 \rangle \left( \sum_i n_i \varepsilon_{0,i} \right)^2 \left( \sum_j \frac{N_b (D_0(\varepsilon_F))^2}{n} \varepsilon_{0,j}^2 \right)
= \frac{\langle \varepsilon_{0x}^2 \rangle D_0(\varepsilon_F)^2 n}{N_b} \left( \sum_i \varepsilon_{0,i} \right) \left( \sum_j \varepsilon_{0,j}^2 \right) \tag{2.87}
$$

if the renormalisation of each of the bands are also equivalent, the factors of $\varepsilon_0$ cancel and $f_{dx;N_b}(n)$ becomes the single band function, Eqn. (2.78), multiplied by the number of bands squared

$$
f_{dx;N_b}(n) = \frac{\langle \varepsilon_{0x}^2 \rangle D_0(\varepsilon_F)^2 n}{N_b} \left( \sum_i \varepsilon_{0,i} \right) \left( \sum_j \varepsilon_{0,j}^2 \right)
= \frac{\langle \varepsilon_{0x}^2 \rangle D_0(\varepsilon_F)^2 n}{N_b} \varepsilon_{0}^2 \left( N_b \varepsilon_{0}^2 \right)
= N_b^2 f_{dx;1}(n). \tag{2.88}
$$

In principle, the general expression, Eqn. (2.86), can be applied to systems of arbitrary band structure to calculate the generalised Kadowaki-Woods ratio, taking into account the effects of band structure. In practice, applying Eqn. (2.86) to realistic systems is performed via density functional theory (or equivalent electronic structure determination techniques), and presents a number of computational complexities, especially in calculating the individual bands’ average squared velocity (which is rarely, if ever, implemented in existing applications). Due to the difficulty involved in such a calculation, the remainder of this work focuses on the application of the generalised Kadowaki-Woods ratio to the two-dimensional semimetal graphene. The relatively simple band structure of graphene allows for analytical calculation of the material-specific quantities, which are identical for each ‘sheet’ in the Fermi surface, and so will combine according to Eqn. (2.88).
3. THE KADOWAKI-WOODS RATIO IN GRAPHENE: PHENOMENOLOGICAL SELF-ENERGY CALCULATION

The behaviour of the dimensionless Kadowaki-Woods ratio in semimetals, materials with extremely low charge carrier densities, where the presence of more than one band is significant to the electronic properties, remains to be examined. As such, the following chapters focus on the examination of the generalised form of the ratio in monolayer graphene, a two-dimensional semimetal material that also possesses a band structure for which the material-specific quantities can be calculated analytically.

Graphene is an interesting material in its own right and the focus of a great deal of experimental and theoretical attention, for a number of reasons, including, for example, the existence of a nonzero conductivity in the undoped regime (i.e. at half filling, where the Fermi surface vanishes) [41–46], anomalously large thermal conductivity (dominated by the phonon contribution) [42–44, 47], and the existence of both anomalous and fractional quantum Hall phases [41–44, 48]. Aside from these, and many other, properties, graphene also exhibits an unusual band structure. In the dispersion of graphene (see Fig. 3.1), there exist ‘cones,’ points in the unit cell with a linear dispersion at low energies (i.e. close to half-filling), with dispersion $\varepsilon_k = \pm \hbar v_F |k|$, with $v_F$ the constant Fermi velocity. Of the six cones, only two are unique, lying within the first unit cell of the reciprocal lattice (the first Brillouin zone). These cones are termed Dirac cones, due to the fact that, with this linear dispersion, electrons behave as though they are massless relativistic particles, as described by the massless Dirac equation (also called the Weyl equation) [42]. As a result, the Fermi ‘surface’ (more accurately the Fermi line in 2D) of graphene has two identical ‘sheets’ (circles, vanishing to points at half-filling), given by each cone where they intersect the Fermi level.

Additionally, in graphene, the electron density, and therefore chemical potential (here used interchangeably with Fermi energy at low temperatures) can be externally controlled. This is achieved either by chemical doping or through the application of a gate voltage to the sample [42, 43]. This allows the control of the transition between the intrinsic (undoped) state of graphene (where the Fermi level lies on the point of the Dirac cones), which is predicted to behave as a marginal Fermi liquid, and the extrinsic (doped) state, which exhibits normal Fermi liquid behaviour [44, 49–51].

As a first estimate of the Kadowaki-Woods ratio in graphene, we assume that the self-energy in graphene has the same phenomenological form as that given previously (Eqn. (2.58)) and, as such, the material-dependent quantities combine as derived in Chapter 2. In doing this, we neglect any changes to the self-energy that arise as a result of the two-dimensional structure of graphene, the treatment of which forms the focus of the next two chapters.

![Fig. 3.1: Electronic dispersion of single-layer graphene, with a Dirac cone highlighted. Reproduced from [42].](image-url)
3. Material Specific Function

We proceed to calculate the material specific function for graphene, \( f_g(n) \), for each individual sheet in the Fermi surface, given the above assumption, that the phenomenological self-energy of Miyake, Matsuura and Varma [34], and therefore the general form of the Kadowaki-Woods ratio, Eqn. (2.88), is valid for graphene.

3.1 Density of States

The (bare) density of states for a system with dispersion given by \( \varepsilon_k \) is defined as [3]

\[
D_0(\varepsilon) = \frac{2}{(2\pi)^2} \int_{BZ} d^2k \delta(\varepsilon - \varepsilon_k),
\]

where the integral is performed over the first Brillouin zone (the primitive unit cell of the lattice in reciprocal space [3]), which gives, for the low-energy graphene dispersion \( \varepsilon_k = \pm \hbar v_F|k| \),

\[
D_0(\varepsilon) = \frac{2}{(2\pi)^2} \int_{BZ} d^2k \delta(\varepsilon - (\pm \hbar v_F |k|)).
\]

The energy delta function can be decomposed into a sum of delta functions of \(|k|\) using the identity [27]

\[
\delta(f(x)) = \sum_{x_0} |\nabla_x f(x)|^{-1} \delta(x - x_0)
\]

where \( x_0 \) are the values of \( x \) that give the roots of \( f(x) \) (i.e. \( f(x_0) = 0 \)). The density of states in graphene is then

\[
D_0(\varepsilon) = \frac{2}{(2\pi)^2} \frac{\hbar v_F}{\pi} \int_{BZ} d^2k \left[ \delta\left(\frac{\varepsilon}{\hbar v_F} - |k|\right) + \delta\left(\frac{\varepsilon}{\hbar v_F} + |k|\right)\right],
\]

where the first (second) delta function corresponds to an energy above (below) the Dirac point (\( \varepsilon = 0 \)), which is the Fermi energy of intrinsic graphene. Given that we are assuming we are in the extrinsic, Fermi liquid, state of graphene, with positive doping, we neglect the second delta function, and the density of states at the Fermi surface becomes

\[
D_0(\varepsilon_F) = \frac{2}{(2\pi)^2} \frac{\hbar v_F}{\pi} \int_{BZ} d^2k \delta(k_F - |k|)
\]

\[
= \frac{2}{(2\pi)^2} \frac{\hbar v_F}{\pi} \int_{BZ} d|k| d\phi |k| \delta(k_F - |k|)
\]

\[
= \frac{k_F}{\pi \hbar v_F}.
\]

The squared density of states at the Fermi energy, which appears in the Kadowaki-Woods ratio, is then,

\[
D_0(\varepsilon_F)^2 = \frac{k_F^2}{(\pi \hbar v_F)^2}
\]

\[
= \frac{n}{\pi (\hbar v_F)^2},
\]

where \( n = \frac{k_F^2}{2\pi} \) [43].

3.1.2 Average Velocity Squared

The (bare) average velocity squared is given by

\[ \langle v_k^2 \rangle = \frac{2}{(2\pi)^2} \int_{BZ} d^2k v_k^2 \delta(\varepsilon - \varepsilon_k) \]

\[ = \frac{2}{(2\pi)^2} D_0 (\varepsilon_F) \int_{BZ} d^2k v_k^2 \delta(\varepsilon - \varepsilon_k) \]

\[ = \frac{2}{(2\pi)^2} D_0 (\varepsilon_F) \int_{BZ} d^2k \rho \left( \frac{1}{\hbar} \nabla_k \varepsilon_k \right) \delta(\varepsilon - \varepsilon_k). \]  (3.7)

The group velocity squared for graphene is given by

\[ \left| \frac{1}{\hbar} \nabla_k \varepsilon_k \right|^2 = \left| \frac{1}{\hbar} \nabla_k \left[ \pm \hbar v_F |k| \right] \right|^2 \]

\[ = \left| \pm \hbar v_F \nabla_k \sqrt{k_x^2 + k_y^2} \right|^2 \]

\[ = v_F^2. \]  (3.8)

At low energies, the graphene dispersion is isotropic around each Dirac point, so that \( \langle v_k^2 \rangle = \langle v_{k,x}^2 \rangle \), and, with the condition \( \langle v_k^2 \rangle = v_F^2 \), this gives

\[ \langle v_k^2 \rangle = \langle v_{k,y}^2 \rangle + \langle v_{k,x}^2 \rangle \]

\[ = v_F^2, \]

\[ \langle v_{k,y}^2 \rangle = \langle v_{k,x}^2 \rangle = \frac{v_F^2}{2}. \]  (3.9)

so that the average velocity in the \( x \)-direction squared, which appears in the Kadowaki-Woods ratio is half the Fermi velocity squared.

3.1.3 \( f_g (n) \)

The full material-specific function for each of the two identical sheets in the Fermi surface of graphene is given by

\[ f_{g,1} (n) = \langle v_{k,x}^2 \rangle D_0^2 (\varepsilon_F)n \]

\[ = \frac{v_F^2}{2} \frac{n}{\pi (\hbar v_F)^2} \]

\[ = \frac{n^2}{2\pi \hbar^2}, \]  (3.10)

and the full, combined material-specific function is

\[ f_{g,2} (n) = N_b f_{g,1} (n) \]

\[ = \frac{2n^2}{\pi \hbar^2}, \]  (3.11)

which depends on the electron density, which can, in principle, be controlled experimentally to test this prediction.

3.2 The Kadowaki-Woods Ratio

Finally, the Kadowaki-Woods ratio in graphene is given by Eqn. (2.76)

\[ A = \frac{81}{4\pi \varepsilon_0 h k_b^4 f_{dx:2}(n)} \]

\[ = \frac{81\hbar}{8\varepsilon_0^2 k_b^4 n^2}. \]  (3.12)
The Kadowaki-Woods ratio calculated for graphene, Eqn. (3.12), is dependent on the square of the electron density, which can be externally controlled experimentally by tuning the chemical potential. As such, this electron density dependence should be easily testable and give a clear experimental verification of the form of the arbitrary band structure Kadowaki-Woods ratio. In practice, however, such an experiment faces great difficulties in measuring the heat capacity for graphene, which is greatly complicated by the structure of monolayer graphene, the single atom thick layer of which is unlikely to affect the conditions inside a calorimeter sufficiently to create a measurable difference. It therefore becomes necessary to define the Kadowaki-Woods ratio in terms of a more measurable quantity, related to the heat capacity, such as the thermal conductivity, a calculation which remains to be performed.

Further, the derivation uses the general form of the Kadowaki-Woods ratio, Eqn. (2.75), which was calculated using the three-dimensional self-energy, as opposed to graphene’s strictly two dimensional nature. It is therefore possible that variations of the two-dimensional self-energy from the three dimensional form may result in corrections to the Kadowaki-Woods ratio. To determine the correct form of the Kadowaki-Woods ratio in graphene, the behaviour of Fermi liquids in two dimensions must be carefully taken into account.

There are several well documented differences between three and two dimensional Fermi liquids, in particular, in the electron-electron scattering rate which defines the imaginary part of the self-energy according to Eqn. (1.8) [33, 52, 53]. The chief difference being that, while in three dimensions the scattering rate is proportional to the square of the temperature, in two dimensions the scattering rate has an extra logarithmic dependence ($\Sigma'' \propto T^2 \log(T)$) [32, 52, 54–57]. The effect of this logarithmic dependence on the Kadowaki-Woods ratio is the focus of Chapters 4 and 5.

While the assumption of a three-dimensional self-energy for graphene clearly neglects its two-dimensional structure, the analysis above may be easily extended to the recently experimentally realised three-dimensional topological Dirac semimetal Cd$_3$As$_2$. Band structure measurements indicate the presence of two three-dimensional Dirac cones [58, 59], so that the preceding analysis need only be extended to three dimensions to be applied to Cd$_3$As$_2$. 
4. ELECTRON-ELECTRON SCATTERING IN TWO DIMENSIONS

To determine the general form for the self-energy in two dimensions, we first wish to calculate the scattering rate, which is related to the imaginary part of the self-energy according to Eqn. (1.8). This will in turn allow us to find the real part of the self-energy from the Kramers-Kronig relations, Eqn. (1.11). In this chapter, we calculate the scattering rate for two common two-dimensional systems: the two-dimensional electron gas, as can be found in semiconductor heterostructures, and the case we are more concerned with, that of the semimetal, monolayer (two-dimensional) graphene. In both cases, the self-energy is expected to deviate from the phenomenological three-dimensional form, Eqn. (2.58), given by Miyake, Matsuura and Varma [34, 49, 54–56, 60].

4.1 Two Dimensional Electron Gas

The two-dimensional electron gas (2DEG) is a system of electrons confined to a two-dimensional plane, usually obtained at the interface of two materials, where electrons may become confined in the direction perpendicular to the surfaces, such as in metal-oxide-semiconductor interfaces (such as those in semiconductor heterostructures, for example, GaAs/Al<sub>x</sub>Ga<sub>1-x</sub>As) [55, 61]. Following Hodges, Smith and Wilkins [62], we find the temperature dependence of the scattering rate for a 2DEG via Fermi’s golden rule, considering scattering of two electrons with momenta \( \mathbf{p}_1 \) and \( \mathbf{p}_2 \) and energies \( \varepsilon_1 \) and \( \varepsilon_2 \) into two unoccupied states with momenta \( \mathbf{p}_1' \) and \( \mathbf{p}_2' \) and energies \( \varepsilon_1' \) and \( \varepsilon_2' \), giving the scattering rate

\[
\frac{1}{\tau} = 2 \sum_{\mathbf{p}_1'} \sum_{\mathbf{p}_2'} \int \frac{d^2\mathbf{p}_2}{(2\pi\hbar)^2} W_n F (\varepsilon_2) n_F (-\varepsilon_1') n_F (-\varepsilon_2') \delta (\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2') \delta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2')
\]

\[
= \frac{2W}{(2\pi\hbar)^2} \int \int d^2\mathbf{p}_2 d^2\mathbf{p}_1' d^2\mathbf{p}_2' F (\varepsilon_2) n_F (-\varepsilon_1') n_F (-\varepsilon_2') \delta (\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1' - \mathbf{p}_2') \delta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2'),
\]

(4.1)

where the factor of two comes from the spin degeneracy, \( W \) is the transition probability which is related to the scattering potential \( W \propto |V_{\text{scat}}|^2 \) with \( V_{\text{scat}} \) the scattering potential, averaged over the circle, and the delta functions ensure conservation of energy and momentum. The integral over \( \mathbf{p}_2' \) is performed to evaluate the momentum delta function, which sets

\[
\varepsilon_2' = \frac{1}{2m} (\mathbf{p}_1 + \mathbf{p}_2 - \mathbf{p}_1')^2
\]

\[
= \frac{1}{2m^*} (p_1^2 + p_2^2 + p_1'^2 + 2p_1 p_2 \cos (\phi_2) - 2p_1 p_2 \cos (\phi_1' - \phi_2) - 2p_1 p_1' \cos (\phi_1')),
\]

(4.2)

where \( \phi_1' \) is the angle between \( \mathbf{p}_1 \) and \( \mathbf{p}_1' \), and \( \phi_2 \) the angle between \( \mathbf{p}_1 \) and \( \mathbf{p}_2 \) (see Figure 4.1). The condition of energy conservation then requires

\[
\varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2' = 0
\]

\[
\varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2' = \varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2' - \frac{1}{2m^*} (p_1^2 + p_2^2 + p_1'^2 + 2p_1 p_2 \cos (\phi_2) - 2p_1 p_2 \cos (\phi_1' - \phi_2) - 2p_1 p_1' \cos (\phi_1'))
\]

\[
= f (\phi_1', \phi_2).
\]

(4.3)

The delta function over the energy variables can then be decomposed into a sum of delta functions, via the identity Eqn. (3.3). Conservation of energy therefore imposes the restriction on the angle \( \phi_1' \),

\[
\delta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1' - \varepsilon_2') = \delta (f (\phi_1', \phi_2)) = \sum_{\phi_0} \left| \frac{df (\phi_1', \phi_2)}{d\phi_1'} \right|^{-1} \delta (\phi_1' - \phi_0),
\]

(4.4)

where \( \phi_0 \) are the zeroes of the energy delta function. The scattering rate integral is now given by

\[
\frac{1}{\tau} = \frac{2W}{(2\pi\hbar)^2} \int dp_2 dp_1' d\phi_1' d\phi_2 p_2 n_F (\varepsilon_2) n_F (-\varepsilon_1') \sum_{\phi_0} \left| \frac{df (\phi_1', \phi_2)}{d\phi_1'} \right|^{-1} \delta (\phi_1' - \phi_0),
\]

(4.5)
As the energies are defined by the free electron dispersion \( \varepsilon_n = \frac{\hbar^2}{2m} k_n^2 \) and \( \varepsilon_4 \) is the only term in \( f(\phi'_1, \phi_2) \) that depends on the restricted angle \( \phi'_1 \) (which arises from the conservation of momentum, Eqn. (4.2)), we can make the substitution \( \frac{df}{d\phi_4} = \frac{dc_4}{d\phi_4} \).

We find \( \frac{dc_4}{d\phi_4} \) and \( \phi_0 \) with the aid of momentum conservation,

\[
\begin{align*}
\phi'_2 &= p_1 + p_2 - p'_1 \\
p^2_2 &= (p_1 + p_2 - p'_1)^2, 
\end{align*}
\]

and conservation of energy,

\[
\frac{p^2_2}{2m^*} = \frac{1}{2m^*} (p^2_1 + p^2_2 - p'^2_1),
\]

which can be combined to give

\[
\begin{align*}
p^2_1 + p^2_2 - p'^2_1 &= p^2_1 + p^2_2 + p'^2_2 + 2p_1 p_2 \cos(\phi_2) - 2p_1 p_2 \cos(\phi'_1 - \phi_2) - 2p_1 p'_1 \cos(\phi'_1), \\
p'^2_1 &= -p_1 p_2 \cos(\phi_2) + p_1 p_2 \cos(\phi'_1 - \phi_2) + p_1 p'_1 \cos(\phi'_1). 
\end{align*}
\]

Using the angle addition and subtraction formulae for the sine and cosine functions [63]

\[
\begin{align*}
\sin(a \pm b) &= \sin(a) \cos(b) \pm \cos(a) \sin(b) \\
\cos(a \pm b) &= \cos(a) \cos(b) \mp \sin(a) \sin(b),
\end{align*}
\]

Eqn. (4.8) can be simplified and expressed in terms of the angle \( \phi'_1 \) and a new angular variable \( u \) defined by \( \tan(u) = \frac{p_1 + p_2 \cos(\phi_2)}{p_2 \sin(\phi_2)} \), independent of \( \phi'_1 \),

\[
\begin{align*}
p'^2_1 &= -p_1 p_2 \cos(\phi_2) + p'_1 p_2 \cos(\phi'_1 - \phi_2) + p_1 p'_1 \cos(\phi'_1) \\
&= -p_1 p_2 \cos(\phi_2) + p'_1 p_2 \cos(\phi'_1) \cos(\phi_2) + \sin(\phi'_1) \sin(\phi_2)] + p_1 p'_1 \cos(\phi'_1) \\
&= p'_1 p_2 \sin(\phi_2) \left[ \sin(\phi'_1) + \cos(\phi'_1) \frac{p_1 + p_2 \cos(\phi_2)}{p_2 \sin(\phi_2)} \right] - p_1 p_2 \cos(\phi_2) \\
&\quad = \frac{p'_1 p_2 \sin(\phi_2)}{\cos(u)} \sin(\phi'_1 + u) - p_1 p_2 \cos(\phi_2). \tag{4.10}
\end{align*}
\]

It is important to note here that \( u \) does not represent any observable physical variable, but is merely a mathematical simplification, used for convenience and, as such, the final result will be independent of \( u \). The expression Eqn. (4.10) can be solved to find the roots \( \phi_0 \) given the constraint of momentum conservation. The derivative of \( p'^2_2 = (p_1 + p_2 - p'_1)^2 \) with respect to the angle
φ' can then also be expressed in terms of φ' and u, to give

\[
\frac{dp'^2}{d\phi'_1} = 2p'_1p_2 \sin (\phi'_1 - \phi_2) + 2p_1p'_2 \sin (\phi'_1)
\]
\[
= 2p'_1p_2 \sin (\phi'_1) \cos (\phi_2) - 2p'_1p_2 \cos (\phi'_1) \sin (\phi_2) + 2p_1p'_2 \sin (\phi'_1)
\]
\[
= -2p'_1p_2 \cos (\phi'_1) \sin (\phi_2) + 2p'_1p_2 \sin (\phi'_1) \sin (\phi_2) \frac{p_1 + p_2 \cos (\phi_2)}{p_2 \sin (\phi_2)}
\]
\[
= -2p'_1p_2 \sin (\phi_2) \cos (\phi'_1) \cos (u) + 2p'_1p_2 \sin (\phi_2) \sin (\phi'_1) \sin (u)
\]
\[
= -2p'_1p_2 \sin (\phi_2) \cos (\phi'_1 + u) / \cos (u).
\]

(4.11)

With the aid of Eqn. (4.10), we can find an expression for the absolute value of the derivative, Eqn. (4.11) (see Appendix A.3.2 for details)

\[
\left| \frac{dp'^2}{d\phi'_1} \right|_{\phi'_1 = \phi_0} = \left[ 4p'_1p_2 \sin^2 (\phi_2) / \cos^2 (u) \cos (\phi'_1 + u) \right]^{1/2}
\]
\[
= \left[ 4p_1^2 \left( p_1^2 + p_2^2 - p_1'^2 \right) - 4p_1^2 p_2^2 \cos^2 (\phi_2) \right]^{1/2},
\]

or, in terms of the total energy ε_i + ε_F, with ε_F the Fermi energy

\[
\left| \frac{dz'_1}{d\phi'_1} \right|_{\phi'_1 = \phi_0} = \frac{1}{2m^*} \left| \frac{dp'^2}{d\phi'_1} \right|_{\phi'_1 = \phi_0}
\]
\[
= \frac{2}{2m^*} \left[ (2m^*)^2 (\epsilon_F + \epsilon'_1) (\epsilon_F + \epsilon_1 + \epsilon_2 - \epsilon'_1) - (2m^*)^2 (\epsilon_F + \epsilon_1) (\epsilon_F + \epsilon_2) \cos (\phi_2) \right]^{1/2}
\]
\[
= \frac{2}{2m^*} \left[ (2m^*)^2 \epsilon_1 (\epsilon_1 + \epsilon_2 - \epsilon'_1) - (2m^*)^2 \epsilon_1 \epsilon_2 + (2m^*)^2 (\epsilon_F + \epsilon_1) (\epsilon_F + \epsilon_2) \sin^2 (\phi_2) \right]^{1/2}
\]
\[
\approx 2 \left[ (\epsilon'_1 - \epsilon_2) (\epsilon_1 - \epsilon'_1) + \epsilon_F^2 \sin^2 (\phi_2) \right]^{1/2}.
\]

(4.13)

(4.14)

We can now rewrite the scattering rate integral by performing the integral over φ'_1

\[
\frac{1}{\tau} = \frac{2W}{(2\pi \hbar^2)} \int d^2p_4 d^2p'_4 d^2p'_2 n_F (\epsilon_2) n_F (\epsilon'_2) \delta (p_1 + p_2 - p'_1 - p'_2) \delta (\epsilon_1 + \epsilon_2 - \epsilon'_1 - \epsilon'_2)
\]
\[
= \frac{2W}{(2\pi \hbar^2)} \int dp_4 dp'_4 d\phi_4 dp'_2 n_F (\epsilon_2) n_F (\epsilon'_2) \delta (\epsilon_1 + \epsilon_2 - \epsilon'_1 - \epsilon'_2) \sum_{\phi_0} \left| \frac{d\phi (\phi'_1, \phi_2)}{d\phi'_1} \right|^{-1} \delta (\phi'_1 - \phi_0)
\]
\[
= \frac{4W}{(2\pi \hbar^2) \epsilon_F} \int dp_4 dp'_4 d\phi_4 dp'_2 n_F (\epsilon_2) n_F (\epsilon'_2) \epsilon_1 - \epsilon_2) \frac{1}{2} \left[ (\epsilon'_1 - \epsilon_2) (\epsilon_1 - \epsilon'_1) + \sin^2 (\phi_2) \right]^{1/2},
\]

(4.15)

which we can simplify further by defining x_1 \equiv \frac{\epsilon_1}{k_T}, x'_1 \equiv \frac{\epsilon'_1}{k_T}, (dx'_1 = \frac{\hbar}{m^* k_T}), and x_2 \equiv \frac{\epsilon_2}{k_T}, (dx_2 = \frac{\hbar}{m^* k_T}) and performing the integral over φ_2,

\[
\frac{1}{\tau} = \frac{4W}{(2\pi \hbar^2) \epsilon_F} (m^* k_T)^2 \int dx'_1 dx_2 n_F (x_2 k_T) n_F (\epsilon'_1 - x_1 - x_2 k_T) T (x'_1 - x_2) (x_1 - x'_1) (k_T)^2 \left[ (x'_1 - x_2) (x_1 - x'_1) (k_T)^2 \right]^{1/2},
\]

(4.16)
and for small $A = \frac{(x'_1 - x_2)(x'_2 - x_1)(\pi k T)^2}{\varepsilon_T^2}$ (i.e. $\varepsilon_T \gg \varepsilon_i, \forall i$), $I(A) \approx \log |A| - \log |A|$, while the integral over Fermi distributions is given by $\int dx' dx_2 n_F (x_2 k_T) n_F (x'_1 - x_1 - x_2) k_b T = \frac{1}{2} \frac{(\pi k T)^2 + x_1^2}{2(1 + e^{-x_1})} = \frac{1}{2} (\pi k T)^2 + x_1^2$ (see [22], Appendix A).

Together, these factors result in a temperature dependence of $(k_b T)^2 \log \left| \frac{k_b T}{\varepsilon_F} \right|$. The scattering rate has the approximate form

$$\frac{1}{\tau} \approx -\frac{2W}{(2\pi \hbar)^4 \varepsilon_F (1 + e^{-\pi x_1^2})} (\pi k b T)^2 \left( \log \left( \frac{k_b T}{\varepsilon_F} \right) - \log(2) + F \left( \frac{\varepsilon_1}{k_b T} \right) \right),$$

(4.17)

$$F(x_1) = \frac{1}{2} n_F (-x_1 k_b T)^{-1} \int dx' dx_2 n_F (x_2 k_b T) n_F (x'_1 - x_1 - x_2) k_b T \log \left| (x'_1 - x_2) (x_1 - x'_1) \right|,$$  

(4.18)

where, in the low temperature, $F(x_1)$ vanishes more rapidly than the other terms, as $\varepsilon_1 \to 0$, and is always small enough that it can be safely neglected in resistivity calculations, where the presence of the derivative of the Fermi distribution restricts the energy range of interest to energies close to the Fermi energy ($\varepsilon_1 \approx 0$). [62]

4.2 Low-Energy Graphene

The temperature dependence of the self-energy of graphene can be calculated via a similar method to that used for the 2DEG, using the linear dispersion of graphene at low energies ($\varepsilon = \pm \hbar v_F |k| = \pm \varepsilon_F |p| = \pm (\varepsilon_F p_F)$). The calculation is complicated by the additional factor $\frac{1 + \nu \cos \phi'}{2}$ in the scattering potential [64] (where $\nu = \pm 1$ for scattering within the conduction band and $\nu = -1$ for scattering between the conduction and valence bands, which is only possible in the intrinsic regime, and, as such, neglected for the extrinsic case studied here) in the integral, which takes into account the overlap of states of the diagonalised tight-binding Hamiltonian. Since $W \propto V_{scatt}^2$, the new factor contributes an angular dependence of $\left( \frac{1 + \nu \cos \phi'}{2} \right)^2$ to the transition probability $W$. In our case, we treat the two cones as bands, as they each contribute a `sheet' to the Fermi surface, to then combine the contributions for each sheet as described in Chapter 2.

The scattering rate integral has the form

$$\frac{1}{\tau} = \frac{2W}{(2\pi \hbar)^4} \int d^2 p_2 d^2 p'_2 d^2 p'_1 n_F (x_2) n_F (-\varepsilon'_1) n_F (-\varepsilon'_2) \left( \frac{1 + \cos \phi'_1}{2} \right)^2 \delta (p_1 + p_2 - p'_1 - p'_2) \delta (\varepsilon_1 + \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2)$$

$$= \frac{2W}{(2\pi \hbar)^4} \int d^2 p_2 d^2 p'_2 d^2 p'_1 (v_F p_2) n_F (x_1) n_F (-v_F p'_1) n_F (-v_F p'_2) \left( \frac{1 + \cos \phi'_1}{2} \right)^2 \delta (p_1 + p_2 - p'_1 - p'_2) \frac{1}{v_F} \delta (p_1 + p_2 - p'_1 - p'_2).$$

(4.19)

Again integrating over $p'_2$ to evaluate the momentum conserving delta function, setting $p'_2 = p_1 + p_2 - p'_1$, giving

$$\frac{1}{\tau} = \frac{2W}{(2\pi \hbar)^4} \int d^2 p_2 d^2 p'_1 n_F (x_2) n_F (-v_F p'_1) n_F (v_F p_2) \left( -v_F \sqrt{\frac{|p_1 + p_2 - p'_1|^2}{2}} \right) \left( \frac{1 + \cos \phi'_1}{2} \right)^2 \delta \left( p_1 + p_2 - p'_1 - \sqrt{\frac{|p_1 + p_2 - p'_1|^2}{2}} \right)$$

$$= \frac{2W}{(2\pi \hbar)^4} \int d^2 p_2 d^2 p'_1 n_F (x_2) n_F (-v_F p'_1) n_F (v_F p_2) \left( -v_F \sqrt{\frac{|p_1 + p_2 - p'_1|^2}{2}} \right) \left( \frac{1 + \cos \phi'_1}{2} \right)^2 \delta (f (\phi'_1, \phi'_2)).$$

The remaining delta function can then be expressed as a delta function of one of the angular variables, as previously, via the delta function decomposition ($\delta (f (\phi)) = \sum_{\phi_0} \left| \frac{df}{d\phi} \right|^{-1} \delta (\phi - \phi_0)$).

Expressing the delta function in terms of $\phi_2$, we have the derivative

$$f (\phi'_1, \phi'_2) = p_1 + p_2 - p'_1 - \sqrt{|p_1 + p_2 - p'_1|^2}$$

$$= p_1 + p_2 - p'_1 - \sqrt{p_1^2 + p_2^2 + p'_1^2 + 2p_1 p_2 \cos \phi_2 - 2p_1 p'_1 \cos \phi'_1 - 2p_1 p_2 \cos (\phi'_1 - \phi'_2)},$$

(4.20)

$$\frac{df}{d\phi_2} = \frac{p_1 p_2 \sin \phi_2 + p'_1 p_2 \sin (\phi'_1 - \phi_2)}{\sqrt{|p_1 + p_2 - p'_1|^2}},$$

(4.21)
and the roots of the function are given by

\[ p_1 + p_2 - p'_1 = \sqrt{|p_1 + p_2 - p'_1|^2} \]
\[ = \sqrt{p_1^2 + p_2^2 + 2p_1p_2 \cos \phi_2 - 2p_1p'_1 \cos \phi'_1 - 2p'_1p_2 \cos (\phi'_1 - \phi_2)} \]
\[ (p_1 + p_2 - p'_1)^2 = p_1^2 + p_2^2 + 2p_1p_2 \cos \phi_2 - 2p_1p'_1 \cos \phi'_1 - 2p'_1p_2 \cos (\phi'_1 - \phi_2) \]
\[ p_1^2 + p_2^2 + 2p_1p_2 - 2p_1p'_1 - 2p'_1p_2 = p_1^2 + p_2^2 + 2p_1p_2 \cos \phi_2 - 2p_1p'_1 \cos \phi'_1 - 2p'_1p_2 \cos (\phi'_1 - \phi_2) \]
\[ 0 = p_1p_2 \cos \phi_2 - p_1p'_1 \cos \phi'_1 - p'_1p_2 \cos (\phi'_1 - \phi_2) - p_1p_2 + p_1p'_1 + p'_1p_2. \] (4.22)

We can then rearrange Eqn. (4.22) and make a similar definition to that of the angular variable \( u \) in the 2DEG case, \( \tan(v) = \frac{p_1 - p'_1 \cos \phi'_1}{p'_1 \sin \phi'_1} \), to obtain

\[ 0 = p_1p_2 \cos \phi_2 - p_1p'_1 \cos \phi'_1 - p'_1p_2 \cos (\phi'_1 - \phi_2) - p_1p_2 + p_1p'_1 + p'_1p_2 \]
\[ = p_1p_2 \cos \phi_2 - p_1p'_1 \cos \phi'_1 - p'_1p_2 \sin \phi'_1 \sin \phi_2 - p_1p_2 + p_1p'_1 + p'_1p_2 \]
\[ = p_2 \cos \phi_2 (p_1 - p'_1 \cos \phi'_1) - p_1p'_1 \cos \phi'_1 - p'_1p_2 \sin \phi'_1 \sin \phi_2 - p_1p_2 + p_1p'_1 + p'_1p_2 \]
\[ = p'_1p_2 \sin \phi'_1 \cos \phi_2 \frac{\sin(v)}{\cos(v)} - p'_1p_2 \sin \phi'_1 \sin \phi_2 \frac{\cos(v)}{\cos(v)} - p_1p'_1 \cos \phi'_1 - p_1p_2 + p_1p'_1 + p'_1p_2 \]
\[ = -p'_1p_2 \sin \phi'_1 \frac{\sin(\phi_2 - v)}{\cos(v)} - p_1p'_1 \cos \phi'_1 + p_1p'_1 + p'_1p_2 \] (4.23)

We can then also express Eqn. (4.21) in terms of this new variable \( v \),

\[ p_1p_2 \sin \phi_2 + p'_1p_2 \sin (\phi'_1 - \phi_2) = p_1p_2 \sin \phi_2 + p'_1p_2 \sin \phi'_1 \cos \phi_2 - p'_1p_2 \cos \phi'_1 \sin \phi_2 \]
\[ = p_2 \sin \phi_2 (p_1 - p'_1 \cos \phi'_1) + p'_1p_2 \sin \phi'_1 \cos \phi_2 \]
\[ = p'_1p_2 \sin \phi'_1 \sin \phi_2 \frac{\sin(v)}{\cos(v)} + p'_1p_2 \sin \phi'_1 \cos \phi_2 \frac{\cos(v)}{\cos(v)} \]
\[ = p'_1p_2 \sin \phi'_1 \frac{\cos(\phi_2 - v)}{\cos(v)} \]
\[ \left| \frac{df}{d\phi_2} \right| = \frac{p_1^2p_2^2 \sin^2 \phi'_1 \cos^2(\phi_2 - v)}{(p_1 + p_2 - p'_1)^2 \cos^2(v)} \frac{1}{(1 + \cos \phi'_1)^4} \] (4.24)

which can be expressed in terms of the result of Eqn. (4.23),

\[ p'_1p_2^2 \sin^2 \phi'_1 \frac{\sin^2(\phi_2 - v)}{\cos^2(v)} = (p_1p'_1 + p'_1p_2 - p_1p'_1 \cos \phi'_1 - p_1p_2)^2 \]
\[ = p_1^2p'_1^2 + p'_1p_2^2 + p'_1p_2^2 \cos^2 \phi'_1 - p_1^2p_2^2 - 2p_1p'_1p_2^2 - 2p'_1p_1^2 \cos \phi'_1 - 2p'_1p_2 \cos \phi'_1 \]
\[ = -2p_1p'_1p_2 \cos \phi'_1 - 2p_1p_2p'_1 \cos \phi'_1 - 2p'_1p_2 \cos \phi'_1 \] (4.25)

Making use of Eqn. (A.49), (see Appendix A.3.2), we have the derivative, combined with the overlap factor,

\[ \frac{p'_1p_2^2 \sin^2 \phi'_1 \cos^2(\phi_2 - v)}{(p_1 + p_2 - p'_1)^2 \cos^2(v) (1 + \cos \phi'_1)^4} = \frac{(-2p_1p'_1p_2 \cos \phi'_1 - 2p_1p_2p'_1 \cos \phi'_1 + 2p_1p'_1p_2 \cos \phi'_1 - 2p'_1p_1^2 \cos \phi'_1)}{(p_1 + p_2 - p'_1)^2 (1 + \cos \phi'_1)^4} \]
\[ + \frac{(-2p_1p'_1p_2 - 2p_1p_2p'_1 + 2p'_1p_1^2)}{(p_1 + p_2 - p'_1)^2 (1 + \cos \phi'_1)^4} \]
\[ \left| \frac{df}{d\phi_2} \right| = \frac{\sqrt{(p_1 + p_2 - p'_1)^2 (1 + \cos \phi'_1)^4}}{p_1p'_1 (1 - \cos \phi'_1) [p_1(p'_1 - 2p_2) + 2p_2(p_1 - p_2) - p_1p'_1 \cos \phi'_1]} \]
\[ = \frac{1}{p'_1} \frac{p_1p'_1}{p_1p'_1} (1 - \cos \phi'_1) \left[ \frac{p_1}{p_1} \left( \frac{p'_1}{p_1} - 2 \frac{p_2}{p_1} \right) + 2 \frac{p_2}{p_1} \left( \frac{p'_1}{p_1} - \frac{p_2}{p_1} \right) - \frac{p_1}{p_1} \frac{p'_1}{p_1} \cos \phi'_1 \right] \] (4.26)
Integrating, we obtain (note, the momenta in Eqn. (4.26) have been rearranged to ensure that the argument of the log term in Eqn. (4.27) is explicitly dimensionless)

$$\int d\phi' \left| \frac{(p_1 + p_2 - p'_1)^2 \cos^2(v) (1 + \cos \phi'_1)^4}{p'_1^2 p'_2 \sin^2 \phi'_1 \cos^2 (\phi_2 - v)} \right|_{f=0}^{1} = \frac{\tan \frac{\phi'}{2} \sqrt{(p_1 - p_2 + p'_1)^2 (1 + \cos \phi'_1)^4}}{\sqrt{1 - \cos \phi'_1} \left( \cos \frac{\phi'}{2} \right)^2}$$

$$\times \left[ \sqrt{(p_1 (2p_2 - p'_1) + 2p_2 (p_2 - p'_1) + p_1 p'_1 \cos \phi'_1)} \right] \left[ \frac{\sqrt{2p_2 (p_1 (p_2 - 3p'_1) + p_2 (p_2 - p'_1)) \log \left[ \frac{\sqrt{2p_2 \sqrt{p'_1 p_2} \cos \frac{\phi'}{2} + \left[ \frac{p_1 p'_1}{p_2} - 2 \frac{p_2}{p_2} + 2 \frac{p_2}{p_2} \left( \frac{p'_1}{p_2} - p_2 - p'_1 \cos \phi'_1 \right)}{2} \right]}\right]}{2 \cos \frac{\phi'}{2} (p_1 p'_1)^2} \right].$$

(4.27)

In the definite integral between 0 and $2\pi$, the $\tanh^{-1}$ term cancels and we are left with

$$\int_0^{2\pi} d\phi' \left| \frac{(p_1 + p_2 - p'_1)^2 \cos^2(v) (1 + \cos \phi'_1)^4}{p'_1^2 p'_2 \sin^2 \phi'_1 \cos^2 (\phi_2 - v)} \right|_{f=0}^{1} = \frac{2 (p_1 + p_2 - p'_1) (p_1 (p_2 - 3p'_1) + p_2 (p_2 - p'_1))}{(p_1 p'_1)^2} \left[ \log \left| -p_1 p'_1 + p_2 (p_1 + p_2 - p'_1) \right| - 2 \log (p_2) + \log (2) \right].$$

(4.28)

Making the change of variables $\varepsilon_n + \varepsilon_F \to v_F n_F$, $d\varepsilon_n \to v_F d n_F$

$$\frac{2 (p_1 + p_2 - p'_1) (p_1 (p_2 - 3p'_1) + p_2 (p_2 - p'_1))}{(p_1 p'_1)^2} \left[ \log \left| -p_1 p'_1 + p_2 (p_1 + p_2 - p'_1) \right| - 2 \log (p_2) + \log (2) \right]$$

$$= \frac{2v_F [\varepsilon_1 + \varepsilon_F + \varepsilon_2 - \varepsilon'_1]}{[\varepsilon_1 + \varepsilon_F + \varepsilon_2 - 3\varepsilon_F + (\varepsilon_2 + \varepsilon_F) (\varepsilon_2 - \varepsilon'_1)]} \left[ \left( \varepsilon_1 + \varepsilon_F \right)^2 \left( \varepsilon_1 + \varepsilon_F \right)^2 - \frac{2 \varepsilon_F \left[ (\varepsilon_1 + \varepsilon_F) (\varepsilon_2 + \varepsilon_F) (\varepsilon_2 - \varepsilon'_1) \right]}{\left( (\varepsilon_1 + \varepsilon_F)^2 \left( \varepsilon_1 + \varepsilon_F \right)^2 \right)} \left[ \log \left| - (\varepsilon_1 + \varepsilon_F) (\varepsilon'_1 + \varepsilon_F) + (\varepsilon_2 + \varepsilon_F) \varepsilon_1 + \varepsilon_F + \varepsilon_2 - \varepsilon'_1 \right| - 2 \log (\varepsilon_F) + \log (2) \right] \right.$$

$$= \frac{2v_F [\varepsilon_1 + \varepsilon_F + \varepsilon_2 - \varepsilon'_1]}{[\varepsilon_1 + \varepsilon_F + \varepsilon_2 - 3\varepsilon_F + (\varepsilon_2 + \varepsilon_F) (\varepsilon_2 - \varepsilon'_1)]} \left[ \left( \varepsilon_1 + \varepsilon_F \right)^2 \left( \varepsilon_1 + \varepsilon_F \right)^2 \right.$$

$$\times \left[ \log \left| \varepsilon_2 (\varepsilon_2 + \varepsilon_1 - \varepsilon'_1) - \varepsilon'_1 (2 \varepsilon_F + \varepsilon_1) \right| - 2 \log (\varepsilon_F) + \log (2) \right].$$

(4.29)

Performing the same change of variables, we can then express the scattering rate in terms of energies

$$\frac{1}{T} = \frac{2W}{v_F (2\pi \hbar)^4} \int d^2 p_2 d^2 p'_1 n_F (v_F p_2) n_F (-v_F p'_1) n_F \left( -v_F \sqrt{p_1 + p_2 - p'_1} \right)^2 \left\{ 1 + \cos \phi'_1 \right\}^2 \frac{\delta (f (\phi'_1, \phi_2))}{2}$$

$$= \frac{2W}{v_F (2\pi \hbar)^4} \int dp_2 dp'_1 d\phi_2 d\phi'_1 n_F (v_F p_2) n_F (-v_F p'_1) n_F \left( -v_F \sqrt{p_1 + p_2 - p'_1} \right)^2 \left\{ 1 + \cos \phi'_1 \right\}^2 \left| \frac{\partial f (\phi'_1, \phi_2)}{\partial \phi_2} \right|^{-1} \delta (\phi_2 - \phi_0)$$

$$= \frac{W}{v_F (2\pi \hbar)^4} \int d\varepsilon_2 d\varepsilon'_1 n_F (\varepsilon_2) n_F (-\varepsilon'_2) n_F \left( -[\varepsilon_1 + \varepsilon_2 - \varepsilon'_1] \right)$$

$$\times (\varepsilon_2 + \varepsilon_F) (\varepsilon'_1 + \varepsilon_F) \left[ \left( \varepsilon_1 + \varepsilon_F + (\varepsilon_2 - \varepsilon'_1) \right) \left( (\varepsilon_1 + \varepsilon_F) (\varepsilon_2 - 3\varepsilon'_1 - 2\varepsilon_F) + (\varepsilon_2 + \varepsilon_F) (\varepsilon_2 - \varepsilon'_1) \right) \right.$$

$$\times \left[ \log \left| \varepsilon_2 (\varepsilon_2 + \varepsilon_1 - \varepsilon'_1) - \varepsilon'_1 (2 \varepsilon_F + \varepsilon_1) \right| - 2 \log (\varepsilon_F) + \log (2) \right].$$

(4.30)
If all energies are close to the Fermi level ($\varepsilon_F \gg \varepsilon_i, \forall i$), we can make the approximation ($\varepsilon_2 - \varepsilon'_1 \approx 0$), which results in the scattering rate

$$
\frac{1}{\tau} \approx \frac{W}{v_F^4 (2\pi \hbar)^4} \int d\varepsilon_2 d\varepsilon'_1 n_F (\varepsilon_2) n_F (-\varepsilon'_1) n_F (-\varepsilon_i + \varepsilon_2 - \varepsilon'_1) \times \left(\varepsilon_2 + \varepsilon_F\right) \left(\varepsilon'_1 + \varepsilon_F\right) \frac{[\varepsilon_1 + \varepsilon_F] - 2(\varepsilon_1 + \varepsilon_F)(\varepsilon'_1 + \varepsilon_F)}{(\varepsilon_1 + \varepsilon_F)^2 (\varepsilon'_1 + \varepsilon_F)^2} \times \left[\log \left|\varepsilon_2 (\varepsilon_2 + \varepsilon_1 - \varepsilon'_1) - \varepsilon'_1 (2\varepsilon_F + \varepsilon_1)\right| - 2 \log (\varepsilon_F) + \log (2)\right]$$

$$
\approx \frac{-2W \varepsilon_F (k_b T)^2}{v_F^4 (2\pi \hbar)^4} \int d\varepsilon_2 d\varepsilon'_1 n_F (\varepsilon_2) n_F (-\varepsilon'_1) n_F (-\varepsilon_2 + \varepsilon'|k_b T) \times \left[\log \left|x_2 (x_2 + x_1 - x'_1) - x'_1 \left(2\frac{\varepsilon_F}{k_b T} + x_1\right)\right| \left(\frac{k_b T}{\varepsilon_F}\right)^2 \left(2 \log (2) + 2 \log \left(\frac{k_b T}{\varepsilon_F}\right)\right)\right].
$$

(4.31)

Making the further substitutions $x'_1 = \frac{\varepsilon'_1}{k_b T}$, $x_1 = \frac{\varepsilon_1}{k_b T}$ and $x_2 = \frac{\varepsilon_2}{k_b T}$, we have

$$
\frac{1}{\tau} \approx \frac{-2W \varepsilon_F (k_b T)^2}{v_F^4 (2\pi \hbar)^4} \int d\varepsilon_2 d\varepsilon'_1 n_F (\varepsilon_2) n_F (-\varepsilon'_1) n_F (-\varepsilon_2 + \varepsilon'|k_b T) \times \left[\log \left|x_2 (x_2 + x_1 - x'_1) - x'_1 \left(2\frac{\varepsilon_F}{k_b T} + x_1\right)\right| \left(\frac{k_b T}{\varepsilon_F}\right)^2 \left(2 \log (2) + 2 \log \left(\frac{k_b T}{\varepsilon_F}\right)\right)\right].
$$

(4.32)

Using the result of Morel and Nozieres (see the appendix of [22]),

$$
\int_{-\infty}^{\infty} d\varepsilon_2 d\varepsilon'_1 n_F (-\varepsilon_2) n_F (-\varepsilon'_1) n_F (-\varepsilon'_2) \delta (\varepsilon_1 - \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2) = \frac{1}{2} \left(\varepsilon_1^2 + (\pi k_b T)^2\right) \frac{1}{1 + e^{-\frac{\varepsilon_1}{k_b T}}},
$$

(4.33)

we can further simplify the scattering rate

$$
\frac{1}{\tau} \approx \frac{-W \varepsilon_F \left(\varepsilon_1^2 + (\pi k_b T)^2\right)}{v_F^4 (2\pi \hbar)^4 (1 + e^{-\beta \varepsilon_1})} \left[\log (2) + 2 \log \left(\frac{k_b T}{\varepsilon_F}\right)\right] - \left[\frac{2W \varepsilon_F (\pi k_b T)^2}{v_F^4 (2\pi \hbar)^4} \int d\varepsilon_2 d\varepsilon'_1 n_F (\varepsilon_2) n_F (-\varepsilon'_1) n_F (-\varepsilon_2 + \varepsilon'|k_b T) \log \left|x_2 (x_2 + x_1 - x'_1) - x'_1 \left(2\frac{\varepsilon_F}{k_b T} + x_1\right)\right| \left(\frac{k_b T}{\varepsilon_F}\right)^2 \left(2 \log (2) + 2 \log \left(\frac{k_b T}{\varepsilon_F}\right)\right)\right].
$$

(4.34)

Again, we have a logarithmic temperature dependence arising in the scattering rate for a two-dimensional system, though, unlike in the 2DEG, this logarithm is not the result of a low-energy approximation (as was made in evaluating the angular integral $I(A)$), but a direct result of the calculation. In the limit $k_b T \gg \varepsilon_1$, Eqn. (4.34) becomes

$$
\lim_{k_b T \gg \varepsilon_1} \frac{1}{\tau} = \frac{-W \varepsilon_F \left(\varepsilon_1^2 + (\pi k_b T)^2\right)}{v_F^4 (2\pi \hbar)^4} \log \left(\frac{\sqrt{2} k_b T}{\varepsilon_F}\right).
$$

(4.35)
4.2.1 The Zero Temperature Limit

We now investigate the zero temperature limit of the monolayer graphene scattering rate, Eqn. (4.34), to determine if the logarithmic factor persists. In the zero temperature limit, we replace the distribution functions with step functions

\[
\frac{1}{\tau} \approx \frac{2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int d\varepsilon_2 d\varepsilon_1' n_F (\varepsilon_2) n_F (-\varepsilon_1') n_F (-\varepsilon_1 + \varepsilon_2 - \varepsilon_1') \times \log \left| \frac{2\varepsilon_2 (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') - \varepsilon_1' (2\varepsilon_F + \varepsilon_1)}{\varepsilon_F^2} \right| \]

\[
\approx \frac{2W\varepsilon_F}{v_F^1 (2\pi\hbar)^4} \int d\varepsilon_2 d\varepsilon_1' \Theta (-\varepsilon_2) \Theta (\varepsilon_1') \Theta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') \times \log \left| \frac{2\varepsilon_2 (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') - \varepsilon_1' (2\varepsilon_F + \varepsilon_1)}{\varepsilon_F^2} \right| \\
\approx \frac{2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int d\varepsilon_2 \int d\varepsilon_1' \Theta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') \times \log \left| \frac{2\varepsilon_2 (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') - \varepsilon_1' (2\varepsilon_F + \varepsilon_1)}{\varepsilon_F^2} \right|.
\]

Making the change of variables \(\varepsilon_2 \rightarrow -\varepsilon_2\), we obtain

\[
\frac{1}{\tau} \approx \frac{2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int_0^\infty d\varepsilon_2 \int_0^{\varepsilon_1} d\varepsilon_1' \Theta (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') \times \log \left| -2\varepsilon_2 (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') + \varepsilon_1' (2\varepsilon_F + \varepsilon_1) \right| \\
\approx \frac{2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int_0^{\varepsilon_1} d\varepsilon_2 \int_0^{\varepsilon_1 - \varepsilon_2} d\varepsilon_1' \log \left| -2\left( \frac{\varepsilon_2 (\varepsilon_1 + \varepsilon_2 - \varepsilon_1') + \varepsilon_1' (2\varepsilon_F + \varepsilon_1)}{\varepsilon_F^2} \right) \right|.
\]

Assuming that all energies are much smaller than the Fermi energy, we take the argument of the logarithm only up to order \(O\left(\frac{1}{\varepsilon_F}\right)\), and the scattering rate is

\[
\frac{1}{\tau} \approx \frac{2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int_0^{\varepsilon_1} d\varepsilon_2 \int_0^{\varepsilon_1 - \varepsilon_2} d\varepsilon_1' \log \left| \frac{4\varepsilon_1'}{\varepsilon_F} \right|,
\]

setting \(E = \varepsilon_1 - \varepsilon_2\),

\[
\frac{1}{\tau} \approx \frac{-2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int_0^{\varepsilon_1} \int_0^E d\varepsilon_1' \log \left| \frac{4\varepsilon_1'}{\varepsilon_F} \right| \\
\approx \frac{-2W\varepsilon_F}{v_F^0 (2\pi\hbar)^4} \int_0^{\varepsilon_1} \int_0^{-E + E \log \frac{4E}{\varepsilon_F}} d\varepsilon_1' \\
\approx \frac{-W\varepsilon_F e_F^2}{v_F^0 (2\pi\hbar)^4} \left( \log \left| \frac{4\varepsilon_1}{\varepsilon_F} \right| - \frac{3}{2} \right),
\]

in agreement with previous calculations, the self-energy, being related to the scattering rate by Eqn. (1.8), \(\Sigma''_{\omega,k} = \frac{-\hbar}{2\pi v_F} \), has a logarithmic dependence on the energy measured from the Fermi energy, at zero temperature [49, 60].
4.3 General Self-Energy in Two Dimensions

The form of the scattering rate in two dimensions has been studied extensively previously \[49, 54–57, 60, 62\]. From our calculations we have the approximate form for a two-dimensional electron gas, (for \(k_bT, \varepsilon_F \gg \varepsilon\))

\[
\Sigma''_{2\text{DEG}} = -\frac{\hbar}{2\tau_{2\text{DEG}}} \approx \frac{\hbar W}{(2\pi\hbar)^4 \varepsilon_F} \left(1 + e^{-\frac{\varepsilon}{k_bT}}\right)^2 \left[(\pi k_b T)^2 + \varepsilon^2\right] \log \left(\frac{k_b T}{2\varepsilon_F}\right),
\]

(4.40)

and for monolayer graphene, at zero temperature (for \(\varepsilon_F \gg \varepsilon\))

\[
\Sigma''_{g,T=0} = -\frac{\hbar}{2\tau_{g,T=0}} \approx \frac{\hbar W \varepsilon_F \varepsilon^2}{2\nu_F^2 (2\pi\hbar)^4} \left(\log \frac{4\varepsilon}{\varepsilon_F}\right),
\]

(4.41)

and at finite temperature (\(k_bT \gg \varepsilon\))

\[
\Sigma''_{g,T \neq 0} \approx \frac{\hbar W \varepsilon_F \left(\varepsilon^2 + (\pi k_b T)^2\right)^2}{2\nu_F^2 (2\pi\hbar)^4} \log \left(\sqrt{2 \frac{k_b T}{\varepsilon_F}}\right).
\]

(4.42)

All of these self-energies are derived in either the low temperature or low energy limit, and solving the scattering rate equations exactly in the intermediate regime (i.e. when the energy and temperature are of comparable magnitudes) is not possible analytically, in general \[9\]. As such, we propose an approximate general form for the imaginary part of the self-energy in two dimensions, which reduces to the above expressions, in the low temperature and low energy regimes, given by

\[
\Sigma''_{\varepsilon,k} = C \left(\varepsilon^2 + (\pi k_b T)^2\right) \log \left(\frac{\sqrt{\varepsilon^2 + (\pi k_b T)^2}}{B\varepsilon_0}\right),
\]

(4.43)

where all energies are measured from the Fermi level, \(B\) is a positive constant of order unity and \(C\) is an (approximately constant) energy scale for the quasiparticle-quasiparticle scattering (in terms of the parameters used in the three dimensional (MMV) self-energy, \(C = \frac{s}{\varepsilon_0}\), where \(s = \frac{\hbar}{k_b}\) is the energy associated with the electron-electron scattering rate and \(\varepsilon_0 \approx Z\varepsilon_F\) is an energy scale characterising the strength of the electron-electron interactions). We also assume that, above the Fermi liquid energy scale, the self-energy decays monotonically, as is assumed in the phenomenological self-energy of Miyake, Matsuura and Varma \[34\]. For graphene and the two-dimensional electron gas, the values of \(B\) and \(C\) are

\[
B_{2\text{DEG}} = \frac{2}{\tau_{2\text{DEG}}},\quad C_{2\text{DEG}} = \frac{\hbar W (m^*)^2}{2(2\pi\hbar)^4 \varepsilon_F},
\]

\[
B_g = \frac{1}{\sqrt{2}},\quad C_g = \frac{\hbar W \varepsilon_F}{2\nu_F^2 (2\pi\hbar)^4},
\]

In the following chapter, we derive the form of the generalised Kadowaki-Woods ratio using the approximate two-dimensional self-energy Eqn. (4.43) and apply the resulting relationship to graphene and calculate the deviation from the value calculated using the three-dimensional self-energy.
5. THE KADOWAKI-WOODS RATIO IN TWO DIMENSIONS:
TWO DIMENSIONAL SELF-ENERGY CALCULATION

Having proposed an approximate form for the self-energy in two dimensions, we focus in this chapter, on the calculation of
the form of the generalised Kadowaki-Woods ratio in two common two-dimensional systems, monolayer graphene and the two-
dimensional electron gas (2DEG).

5.1 Resistivity Coefficient

We wish to determine the coefficient of the quadratic term in the resistivity, given in three dimensions by the formula [3]
\[
\rho(T) = \rho_0 + A T^2. \tag{5.1}
\]

In two dimensions, however, the scattering rate no longer scales quadratically with temperature, but scales as
\[ T^2 \log(T), \]
and, as such, we postulate that the resistivity will follow the relationship
\[
\rho(T) = \rho_0 + A' T^2 \log \left( \frac{T}{T^*} \right), \tag{5.2}
\]
where \( k_b T^* = \frac{B \epsilon_0}{\pi} \), in terms of the parameters of the self-energy. To find \( A' \), we use the result of the Kubo formula calculation
in Chapter 2, in the two-dimensional case, which gives,
\[
\sigma^{(0)}_{xx}(T) = e^2 \hbar \langle v_x^2 \rangle \int_{-\infty}^{\infty} \frac{d^2 k}{(2\pi)^2} Z \delta(\varepsilon_F - Z \varepsilon_k) \int_{-\infty}^{\infty} d \epsilon \left( -\frac{1}{\Sigma'_{\epsilon,k}} \right) \left( -\frac{dn_f(\epsilon)}{d\epsilon} \right). \tag{5.3}
\]
The momentum integral again gives the bare density of states at the Fermi level, assuming the self-energy is independent of \( k \)
\[
\sigma_{xx}(T) = e^2 \hbar \langle v_x^2 \rangle \int_{-\infty}^{\infty} \frac{d^2 k}{(2\pi)^2} \delta(\varepsilon_F - \varepsilon_k) \int_{-\infty}^{\infty} d \epsilon \left( -1 \right) \left( -\frac{dn_f(\epsilon)}{d\epsilon} \right) \tag{5.4}
\]
Taking the derivative of the distribution function, as in Chapter 2 \(-\frac{dn_f(\epsilon)}{d\epsilon} = \frac{1}{4k_b T} \text{sech}^2 \left( \frac{x}{2} \right), \; x = \frac{\varepsilon - \varepsilon_F}{k_b T} \), we have the integral over energy,
\[
\int_{-\infty}^{\infty} dx \left( -\frac{1}{\Sigma'_{\epsilon,k}} \right) \frac{\text{sech}^2 \left( \frac{x}{2} \right)}{4k_b T} = C^{-1} \frac{1}{4 \left( \frac{B \epsilon_0}{k_b T} \right)^2} \int_{-\infty}^{\infty} dx \left( \frac{\text{sech}^2 \left( \frac{x}{2} \right)}{\left( x^2 + \pi^2 \right)} \right) \left( \log \left( \frac{\sqrt{x^2 + \pi^2}}{\left( \frac{B \epsilon_0}{k_b T} \right)} \right) \right)^{-1}, \tag{5.5}
\]
which can then be evaluated with the knowledge that, for low temperatures and \( \frac{B \epsilon_0}{k_b T} \gg \varepsilon, \left( \frac{\text{sech}^2 \left( \frac{x}{2} \right)}{\left( x^2 + \pi^2 \right)} \right) \) is sharply peaked about
\( x = 0 \) (becoming a delta function as \( T \rightarrow 0 \), and \( \left( \log \left( \frac{\sqrt{x^2 + \pi^2}}{\left( \frac{B \epsilon_0}{k_b T} \right)} \right) \right)^{-1} \) varies slowly with \( x \) over the range in which \( \left( \frac{\text{sech}^2 \left( \frac{x}{2} \right)}{\left( x^2 + \pi^2 \right)} \right) \) is
nonzero. Because of this, the factor of \( \left( \log \left( \frac{\sqrt{x^2 + \pi^2}}{\varepsilon_0} \right) \right)^{-1} \) can be approximated by its value at the Fermi energy. The remaining integral gives a factor of \( \frac{1}{3} \), and the final result is

\[
\sigma_{xx}(T) = \frac{e^2 \hbar (v_x^2) D_0 (\varepsilon_F)}{24 C (k_b T)^2} \left( \frac{1}{\log \left( \frac{\pi k_b T}{B \varepsilon_0} \right)} \right). \tag{5.6}
\]

The coefficient \( A' \) in a single band can then be calculated by

\[
A'_{2D} = \frac{1}{T^2 \log \left( \frac{T}{T^*} \right)} \left( [\sigma_{xx}(T)]^{-1} - [\sigma_{xx}(T = 0)]^{-1} \right)
= \frac{24 C k_b^2}{e^2 \hbar (v_x^2) D_0 (\varepsilon_F)}. \tag{5.7}
\]

and the value for \( A' \) in graphene is the sum in parallel of the two identical bands’ \( A' \) values, which gives

\[
A'_g = \frac{A'_{2D}}{2} = \frac{12 C k_b^2}{e^2 \hbar (v_x^2) D_0 (\varepsilon_F)}. \tag{5.8}
\]

### 5.2 Heat Capacity

To find the real part of the self-energy we again utilise the Kramers-Kronig relations [27]

\[
\Sigma''(\varepsilon) = \frac{1}{\pi P} \int_{-\infty}^{\infty} d\varepsilon' \frac{\Sigma''(\varepsilon')}{\varepsilon' - \varepsilon}. \tag{5.9}
\]

To perform the integral over all energies, we assume that the imaginary part of the self-energy in two dimensions obeys Eqn. (4.43) at energies below some cut-off energy (which we will denote \( \varepsilon_0 \) for continuity with the case of Chapter 2), and that above this energy the self-energy is monotonically decreasing, according to some function \( F \left( \frac{\varepsilon^2 + (\pi k_b T)^2}{\varepsilon_0} \right) \) which decreases from \( F(1) = 1 \) to \( F(\infty) = 0 \). In this case, the full form of the imaginary part of the self-energy is

\[
\Sigma''(\varepsilon) = C \left( \frac{\varepsilon^2 + (\pi k_b T)^2}{\varepsilon_0} \right) \log \left( \frac{\varepsilon^2 + (\pi k_b T)^2}{B \varepsilon_0} \right) \quad \text{for } \varepsilon^2 + (\pi k_b T)^2 < \varepsilon_0^2,
= C \varepsilon_0^2 \log \left( \frac{1}{B} \right) F \left( \frac{\varepsilon^2 + (\pi k_b T)^2}{\varepsilon_0^2} \right) \quad \text{for } \varepsilon^2 + (\pi k_b T)^2 > \varepsilon_0^2, \tag{5.10}
\]

with the prefactor of the second equality ensuring the self-energy is continuous at \( \varepsilon = \varepsilon_0 \). We also assume that the pole occurs in the energy range \( |\varepsilon'| \leq \varepsilon_0 \), so the principle part of the integral need only be taken in this range. The zero temperature limit of the real part of the self-energy is then given by

\[
\Sigma'(\varepsilon) = \frac{C}{\pi} \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon' \frac{\varepsilon'^2 \log \left( \frac{\varepsilon'}{\varepsilon_0} \right)}{\varepsilon' - \varepsilon}
+ C \varepsilon_0^2 \log \left( \frac{1}{B} \right) \int_{\varepsilon_0}^{\infty} d\varepsilon' \frac{F \left( \frac{\varepsilon'^2}{\varepsilon_0^2} \right)}{\varepsilon' - \varepsilon}
+ C \varepsilon_0^2 \log \left( \frac{1}{B} \right) \int_{-\infty}^{-\varepsilon_0} d\varepsilon' \frac{F \left( \frac{\varepsilon'^2}{\varepsilon_0^2} \right)}{\varepsilon' - \varepsilon}, \tag{5.11}
\]

\[
\Sigma'(\varepsilon) = I_1 + I_2 + I_3. \tag{5.12}
\]
The second and third terms are proportional to the corresponding integrals already evaluated for the three dimensional case (Eqn. (2.67)), and result in

\[ I_2 + I_3 = 2 \left( \frac{C \varepsilon_0 \log \left( \frac{1}{\beta} \right) \xi}{\pi} \right) \varepsilon, \]

\[ 0 \leq \xi = \int_1^{\infty} dy' F[y] \sum_{n=1}^{\infty} \frac{y^{2(n-1)}}{y^{2n}} \leq 1. \]

The first integral, \( I_1 \), in Eqn. (5.12) is more complicated, and to solve it we first make the change of variables \( \omega = \varepsilon' - \varepsilon \) to move the singularity to the origin,

\[
\frac{C}{\pi} P \int_{-\varepsilon_0}^{\varepsilon_0} d\varepsilon' \frac{\varepsilon'^2 \log \left( \frac{\varepsilon'}{B\varepsilon_0} \right)}{\varepsilon' - \varepsilon} = \frac{C}{\pi} P \int_{-\varepsilon_0}^{\varepsilon_0} d\omega \frac{(\omega + \varepsilon)^2 \log \left( \frac{\omega + \varepsilon}{B\varepsilon_0} \right)}{\omega} = \frac{C}{\pi} P \int_{-\varepsilon_0}^{\varepsilon_0} d\omega \frac{(\omega^2 + 2\omega\varepsilon + \varepsilon^2) \log \left( \frac{\omega + \varepsilon}{B\varepsilon_0} \right)}{\omega},
\]

(5.13)

This integral can then be solved analytically and the resulting expression for the principle part is

\[
P \int_{-\varepsilon_0}^{\varepsilon_0} d\omega \frac{(\omega^2 + 2\omega\varepsilon + \varepsilon^2) \log \left( \frac{\omega + \varepsilon}{B\varepsilon_0} \right)}{\omega} = \lim_{\delta \to 0} \frac{1}{4} \left[ 2\varepsilon^2 \left( 1 - 2 \log(\omega) \right) \log \left( \frac{\varepsilon + \omega}{\varepsilon} \right) - (3\varepsilon + \omega)^2 + 2 \left( 2\varepsilon^2 + 4\varepsilon\omega + \omega^2 + 2\varepsilon^2 \log(\omega) \right) \log \left( \frac{\varepsilon + \omega}{B\varepsilon_0} \right) + 4\varepsilon^2 \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| \right]^{\varepsilon_0 - \varepsilon}
\]

\[ + \left[ 2\varepsilon^2 \left( 1 - 2 \log(\omega) \right) \log \left( \frac{\varepsilon + \omega}{\varepsilon} \right) - (3\varepsilon + \omega)^2 + 2 \left( 2\varepsilon^2 + 4\varepsilon\omega + \omega^2 + 2\varepsilon^2 \log(\omega) \right) \log \left( \frac{\varepsilon + \omega}{B\varepsilon_0} \right) + 4\varepsilon^2 \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| \right]^{-\varepsilon - \varepsilon_0},
\]

(5.14)

where the final \( 4\varepsilon^2 \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| \) term arises from the integral (with the absolute value of the logarithm argument explicitly stated here for clarity)

\[
\int d\omega \frac{\varepsilon^2}{\omega} \log \left| \frac{\omega + \varepsilon}{\varepsilon_0} \right| = \int d\omega \frac{\varepsilon^2}{\omega} \log \left| \frac{\varepsilon}{\varepsilon_0} \right| + \log \left| 1 + \omega\varepsilon^{-1} \right|.
\]

Performing the change of variable \( q = \frac{\varepsilon}{\varepsilon_0} \) on the second term of the integrand gives

\[
\int d\omega \frac{\varepsilon^2}{\omega} \log \left| \frac{\omega + \varepsilon}{\varepsilon_0} \right| = \int d\omega \frac{\varepsilon^2}{\omega} \log \left| \frac{\varepsilon}{\varepsilon_0} \right| + \int dq \frac{\varepsilon^2}{q} \log \left| 1 - q \right|.
\]

with this definition, we have

\[
\lim_{\delta \to 0} \left[ \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| + \int_0^{\delta} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| + \int_0^{\frac{\delta}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| - \int_0^{\frac{\varepsilon_0}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| \right]
\]

\[ = \lim_{\delta \to 0} \left[ \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| + \int_0^{\frac{\delta}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right| \right] \quad \text{or} \quad \int_0^{\frac{-\omega}{t}} \frac{dt}{t} \log \left| 1 - \frac{t}{t} \right|,
\]

(5.15)
The quasiparticle weight is then given by
\[ \frac{1}{2} \varepsilon \left[ 4 \varepsilon_0 \left( \log \left( \frac{1}{B} \right) - 1 \right) + \varepsilon \left( 2 \log [-\varepsilon - \varepsilon_0] - 1 \right) \right] \]
for graphene, \( B \) vanishes. The remaining terms give
\[ \varepsilon \left( 2 \log \left( \frac{\varepsilon_0}{\varepsilon} \right) + 2 \log \left( \frac{\varepsilon_0}{\varepsilon - \varepsilon_0} \right) \right) \]
so, for the real part of the self-energy we have the final expression
\[ \Sigma'_\varepsilon = - \frac{2C\varepsilon_0}{\pi} [(1 + \epsilon) \log (B) + 1] \varepsilon + \mathcal{O}(\varepsilon^3). \] (5.17)

The quasiparticle weight is then given by
\[ Z = \frac{1}{1 + 2C\varepsilon_0 \left( 1 + \epsilon \log (B) + 1 \right)}, \] (5.18)
and the linear heat capacity coefficient \( \gamma \) for each individual two dimensional band is
\[ \gamma = \frac{\pi^2 k_B^2 D_0(\varepsilon_F)}{3} \]
\[ = \frac{\pi^2 k_B^2 D_0(\varepsilon_F)}{3} \left( 1 + 2C\varepsilon_0 \left( 1 + \epsilon \log (B) + 1 \right) \right), \] (5.19)
which takes the approximate value (assuming \( 2C\varepsilon_0 \left( 1 + \epsilon \log (B) + 1 \right) \gg 1 \), and taking the maximum limiting value for \( \epsilon, \xi = 1 \),
\[ \gamma_{2D} = \frac{4\pi k_B^2 D_0(\varepsilon_F) C\varepsilon_0}{3} \left( \log (B) + \frac{1}{2} \right), \] (5.20)
and, for graphene, the \( \gamma \) value is just the sum of the two identical bands’ \( \gamma \) coefficients,
\[ \gamma_g = 2\gamma_{2D} = \frac{8\pi k_B^2 D_0(\varepsilon_F) C\varepsilon_0}{3} \left( \log (B) + \frac{1}{2} \right), \] (5.21)
with \( n_a \), which appears in \( C \), given by \( n_a = \frac{n}{2} \) in terms of the total electron density \( n \).

### 5.3 The Kadowaki-Woods Ratio in Graphene

So, from Eqns. (5.8) and (5.21), we arrive at the two-dimensional Kadowaki-Woods ratio for graphene,
\[ R_{KW} = A' = A' = \frac{A'}{\gamma^2} \]
\[ = \frac{108}{64 \pi^2 k_B^2 h (v_F^2) C \varepsilon_0^2} \frac{1}{\left( D_0(\varepsilon_F) \right)^2} \left( \log (B) + \frac{1}{2} \right)^2 \]
\[ = \frac{1}{4 \pi^2 k_B^2 f_g(n)}, \] (5.22)
\[ f_g(n) = 12 \pi (v_F^2) C \varepsilon_0^2 \left( D_0(\varepsilon_F) \right)^3 \left( \log (B) + \frac{1}{2} \right)^2, \] (5.23)
where, remembering that \( C \sim \frac{\xi}{\varepsilon_0} \), our final value is independent of the value of \( \varepsilon_0 \). In the following section we calculate, for comparison, the Kadowaki-Woods ratio in a 2DEG, for which a greater volume of experimental data is available.

#### 5.3.1 The Two-Dimensional Correction to the Material Specific Function

Evaluating the material dependent factors in \( f_g(n) \), for \( C = \frac{2n}{\varepsilon_0} = \frac{2n_a}{3 \pi \varepsilon_0 D_0(\varepsilon_F) \varepsilon_0^2} = \frac{n}{3 \pi \varepsilon_0 D_0(\varepsilon_F) \varepsilon_0^2} \), gives
\[ f_g(n) = 12 \pi (v_F^2) \left( \frac{n}{3 \pi \varepsilon_0 D_0(\varepsilon_F) \varepsilon_0^2} \right) \varepsilon_0^2 \left( D_0(\varepsilon_F) \right)^3 \left( \log (B) + \frac{1}{2} \right)^2 \]
\[ = 4 (v_F^2) n \left( D_0(\varepsilon_F) \right)^2 \left( \log (B) + \frac{1}{2} \right)^2 \]
\[ = \frac{2n^2}{\pi \hbar^2} \left( \log (B) + \frac{1}{2} \right)^2, \] (5.24)
where the two-dimensional treatment has resulted in the correction \( \left( \log (B) + \frac{1}{2} \right)^2 \) to the value calculated in Chapter 3, where, for graphene, \( B_g = \frac{1}{\sqrt{2}} \), and the Kadowaki-Woods ratio still varies quadratically with the (controllable) electron density.
5.4 The Kadowaki-Woods Ratio in a Two-Dimensional Electron Gas

We calculate here the generalised Kadowaki-Woods ratio for a two-dimensional electron gas, using the two-dimensional form of the resistivity and heat capacity coefficient expressions, Eqs. (5.7) and (5.20),

\[ R_{KW} = \frac{A'}{\gamma^2} = \frac{81}{4\pi^2 c^2 k_b^4 \hbar^2} \frac{\gamma^2}{\epsilon_0^2 [D_0(\epsilon_F)]^3} \frac{2}{3} \frac{1}{(\log (B) + \frac{1}{2})^2} \]

\[ = \frac{81}{4\pi^2 c^2 k_b^4 f_{2DEG} (n)} \]

\[ f_{2DEG} (n) = \frac{3\pi}{2} \langle v_x^2 \rangle [D_0(\epsilon_F)]^3 \left( \log (B) + \frac{1}{2} \right)^2 \]

\[ = \langle v_x^2 \rangle n [D_0(\epsilon_F)]^2 \left( \log (B) + \frac{1}{2} \right)^2, \]

(5.26)

where the density of states at the Fermi surface is

\[ D_0(\epsilon_F) = \frac{2}{(2\pi)^2} \int_{BZ} d^2 k \delta (\epsilon_F - \epsilon_k) \]

\[ = \frac{2}{(2\pi)^2} \int_{BZ} d^2 k \delta \left( \epsilon_F - \frac{\hbar^2 k^2}{2m^*} \right) \]

\[ = \frac{2m}{\pi \hbar^2} \int_{BZ} d |k| |k| \frac{1}{2} |k| \delta (\pm k_F - |k|) \]

\[ = \frac{m}{\pi \hbar^2}, \]

(5.27)

with the density of states squared

\[ (D_0(\epsilon))^2 = \frac{m^2}{\pi^2 \hbar^4}. \]

(5.28)

The average velocity squared for a 2DEG is

\[ \langle v_k^2 \rangle = \frac{2}{(2\pi)^2} D_0(\epsilon_F) \int_{BZ} d^2 k v_{k,x}^2 \delta (\epsilon_F - \epsilon_k), \]

where the velocity \( v_{k,x} \) is the electron group velocity, \( \frac{1}{\hbar} \nabla_k \epsilon_k \), and the energy is given by the parabolic dispersion \( \epsilon_k = \frac{\hbar^2 k^2}{2m^*} \).

The average velocity squared is then

\[ \langle v_x^2 \rangle = \frac{2}{(2\pi)^2} D_0(\epsilon_F) \int_{BZ} d^2 k v_{k,x}^2 \delta (\epsilon_F - \epsilon_k) \left( \frac{\hbar^2 k^2}{2m^*} \right) \]

\[ = \frac{2}{(2\pi)^2} D_0(\epsilon_F) \frac{2m}{\hbar^2} \int_{BZ} d^2 k \frac{h^2 k^2}{m^2} \delta (k_F^2 - k^2) \]

\[ = \frac{2}{\pi D_0(\epsilon_F)} \int_{BZ} d |k| |k| \frac{1}{2} |k| \frac{m^2}{2} \delta (k_F^2 - |k|) \]

\[ = \frac{k_F^2}{\pi m D_0(\epsilon_F)} = \frac{h^2 k_F^2}{m^2} = v_F^2. \]

(5.29)

Using again the isotropic nature of the dispersion at low energies, we have the average squared velocity in the \( x \)-direction,

\[ \langle v_{k,x}^2 \rangle = \frac{v_F^2}{2} = \frac{h^2 k_F^2}{2m^2}. \]

(5.30)
The material-specific function for a 2DEG is then given by Eqn. (5.26),
\[
J_{2DEG}(n) = \langle v_F^2 \rangle n [D_0(\varepsilon_F)]^2 \left( \log (B) + \frac{1}{2} \right)^2
\]
\[
= \frac{k_F^2 n}{2m^2} \frac{2n^2}{\pi^2 \hbar^4} \left( \log (B) + \frac{1}{2} \right)^2
\]
\[
= \frac{k_F^2}{2\pi^2 \hbar^4} n \left( \log (B) + \frac{1}{2} \right)^2 = \frac{n^2}{\pi \hbar^2} \left( \log \left( \frac{2n}{k_F^2} \right) + \frac{1}{2} \right)^2,
\] (5.31)

where we have used the expression for the electron density of a 2DEG, \( n = \frac{k_F^2}{2\pi^2} \), and, for the 2DEG, \( B_{2DEG} = 2 \). We find that the value of the Kadowaki-Woods ratio for the two-dimensional electron gas differs from the value calculated for graphene by a factor of 2, with the same quadratic dependence on the electron density.

5.5 Resistivity and the Logarithmic Temperature Dependence

In deriving the two-dimensional Kadowaki-Woods ratio, Eqn. (5.22), we have calculated the scattering rate via Fermi’s golden rule, invoking conservation of (crystal) momentum. Intuitively, this presents the troubling question of how relaxation occurs when (crystal) momentum is conserved. The simplest answer to this question is that relaxation occurs because it is the quasimomentum, or crystal momentum \((\hbar \mathbf{k})\), that is conserved, as opposed to the true momentum. Since the crystal momentum is the conserved quantity and is only defined up to a primitive lattice vector in the reciprocal lattice, there exist scattering processes which conserve the total momentum but only conserve crystal momentum modulo a reciprocal lattice vector, with some momentum transfer to the lattice [3]. These are known as Umklapp processes and these processes, even when not the dominant scattering processes, are sufficient to relax the momenta and result in a nonzero resistivity [4].

The conditions for Umklapp scattering are, however, fairly strict. Aside from broken continuous translational symmetry, as is present in any periodic lattice, the carrier density is also a factor. Umklapp processes can only occur if the total (real) momentum transfer is equal to or greater than a primitive reciprocal lattice vector. For quasiparticle-quasiparticle scattering, this condition is equivalent to the Fermi surface occupying at least a quarter of the first Brillouin zone. In many materials the Fermi surface is much smaller than the minimum required for quasiparticle-quasiparticle Umklapp processes, and yet a quadratic temperature dependence is still found experimentally in the resistivity. Pal, Yudson and Maslov (PYM) [65] offer a potential answer to how this is possible. The important distinction, they argue, is that in periodic systems, momentum conservation does not imply velocity conservation, as periodic systems do not necessarily preserve Galilean invariance, and the velocity \( \mathbf{v}_k \) and wavevector \( \mathbf{k} \) are therefore not necessarily parallel, in general. PYM go on to perform a calculation of the resistivity in a material dominated by impurity scattering, by treating the quasiparticle-quasiparticle scattering as a perturbation to the total scattering rate. They find that a quadratic temperature dependence exists even in such systems at close to zero temperature.

While the logarithmic temperature dependence of the resistivity in two dimensions would seem to be a straightforward conclusion from the form of the scattering rate, there is considerable uncertainty, motivated by a lack of experimental confirmation, regarding whether this straightforward approach is accurate. The perturbative calculation of Pal, Yudson and Maslov finds no logarithmic contribution to the resistivity to lowest order in the quasiparticle-quasiparticle interaction in two dimensions. This result becomes invalid, however, in materials with a low impurity concentration, where the perturbative treatment of quasiparticle-quasiparticle scattering is no longer reasonable. At higher orders in the perturbation, PYM do indeed see a logarithmic temperature dependence arise.

At present, there is a lack of experimental evidence for the existence of a logarithmic temperature dependence in the two dimensional resistivity, which follows from the form of the scattering rate in two dimensions. In part this may arise from the size of the logarithmic correction, which may be difficult to observe, as can be seen in Fig. 5.1. We have deliberately imposed no restrictions on the size of the parameter \( B \) of the general two-dimensional self-energy, Eqn. (4.43). As a result, we can say little about the size of this logarithmic correction. However, the deviation of the Kadowaki-Woods ratio calculated with the logarithmic correction to the self-energy (Eqn. (5.24)) from that calculated without the correction (Eqn. (3.12)),
\[
\frac{A'}{\gamma^2} = \frac{A}{\gamma^2} \left( \log (B) + \frac{1}{2} \right)^2,
\] (5.32)
could potentially give an indirect experimental probe of the size of \( B \) and the presence of a logarithmic temperature dependence in the resistivity.
Fig. 5.1: To create this figure, we have randomly generated ‘resistivity’ data points, distributed according to $\rho = T^2 \log(T)$ over more than three orders of magnitude (with random experimental uncertainty ($\leq 1\%$)), and plotted the logarithm of the ‘resistivity’ against the logarithm of the ‘temperature’. The resulting plot is very close to linear, what one might expect from a quadratic temperature dependence in the resistivity without the additional logarithmic factor. For a resistivity that depends on temperature according to $\rho = AT^2$, one expects a linear regression $y = 2x + c$ where $y = \log(\rho)$, $x = \log(T)$, $c = \log(A)$. The variation of the regression line gradient from the expected value could potentially be explained by a nonzero residual (impurity) resistivity, or experimental uncertainty. As such, it can be understood that the logarithmic temperature dependence may be difficult to detect experimentally, unless the logarithmic correction is very large.
We have derived a generalised expression of the dimensionless Kadowaki-Woods ratio in systems of arbitrary band structure, which accounts for possible variations in the value of the ratio due to the presence of multiple bands and non-spherical Fermi surfaces. This calculation lead to the clear implication that, in a system of multiple bands, the Kadowaki-Woods ratio has a clear dependence on both the number and properties of the individual bands, and the simple model of Jacko, Fjærestad and Powell will not give the exact value. The derivation has also resulted in the analytical tools required to combine the various bands’ contributions to the Kadowaki-Woods ratio. Taking the effects of band structure into account, divergences of the Kadowaki-Woods ratio should then only occur as a result of non-Fermi liquid behaviour or the presence of significant vertex corrections (which may become non-negligible near magnetic quantum critical points [13, 66, 67]).

To determine these individual band contributions in general, however, one needs to make use of electronic structure calculation techniques (e.g. density functional theory), which must be heavily modified to give the desired quantities. Due to the complexity of implementing such methods, our further analysis was restricted to analytically tractable systems, in particular monolayer graphene, for which calculations of the band contributions can be performed without the need for computational electronic structure determination.

We have then applied the Kadowaki-Woods ratio to the two-dimensional semimetal graphene, first by assuming that the general phenomenological Fermi liquid self-energy used in the derivation of the general form of the Kadowaki-Woods ratio is valid for graphene. This allowed the result of Chapter 2 to be applied directly to graphene, which yielded a Kadowaki-Woods ratio with a simple quadratic dependence on the charge carrier density. This, in turn, may facilitate future investigations of the behaviour of the Kadowaki-Woods ratio in low carrier density systems, and presents a potential test for the validity of the result, as the carrier density in graphene may be externally controlled and varied continuously via doping or the application of an external gate voltage.

Though calculated here in the context of two-dimensional graphene, for which the three-dimensional form of the self-energy is not necessarily applicable, this analysis can be extended straightforwardly to the recently identified three-dimensional topological Dirac semimetal, Cd$_3$As$_2$ [58, 59]. Referred to as a three-dimensional analogue of graphene, this compound exhibits a band structure strikingly similar to that of graphene, in particular the existence of two three-dimensional Dirac cones. As such, the derivation of the Kadowaki-Woods ratio of Chapter 3 need only be modified slightly to be applied to Cd$_3$As$_2$.

We then addressed the additional complexities that arise in two dimensional systems such as graphene and the two-dimensional electron gas, where the self-energy may vary from the form used in the derivation of the generalised Kadowaki-Woods ratio. We found that, if the experimentally elusive ‘2D log’ contribution is included in the self-energy, it does not effect the dependence of the ratio on carrier density, but results in an additional factor. This factor, if measured, could give indirect evidence for the existence of the logarithmic temperature dependence of the self-energy and therefore resistivity.

In summary, we have derived a generalisation of the dimensionless Kadowaki-Woods ratio which takes into account the possibility of complex arbitrary band structures and their effects on the ratio via a simple relationship (Eqn. 2.86). We have then applied this relationship to the analytically solvable two-dimensional semimetal graphene, taking into account the effects of reduced dimensionality. In doing so, we have found that the Kadowaki-Woods ratio has a simple quadratic dependence on the externally controllable charge carrier density, and that the effects of reduced dimension manifest in a correction to the magnitude of the ratio, which may itself prove an indirect test for the proposed logarithmic temperature dependence of the resistivity in two dimensions.
APPENDIX
A. APPENDIX

A.1 Derivation of the Universal Kadowaki-Woods Ratio for One Band Systems

A.1.1 Resistivity

In this section, we first derive the form of the quadratic resistivity coefficient in single band systems, the \( N_b = 1 \) limit of the derivation of Chapter 2, included here for completeness, following [6] Section 8.1, pp. 505-508 closely.

An expression for the conductivity of a material can be found from the current-current correlation function. We first define the interaction Hamiltonian, with \( c \) and \( c^\dagger \) the usual fermion annihilation and creation operators,

\[
H = H_0 + V, \tag{A.1}
\]

\[
H_0 = \sum_{p,\sigma} \xi_{p,\sigma} c_{p,\sigma}^\dagger c_{p,\sigma}, \tag{A.2}
\]

and the component of the current density operator in the direction \( \alpha \) defined as

\[
j_{\alpha} = e \sum_{p,\sigma} v_{p,\sigma,\alpha} c_{p,\sigma}^\dagger c_{p,\sigma}, \tag{A.3}
\]

where \( e \) is the charge of an electron, \( v_{p,\alpha} = \nabla_p \varepsilon_p = \frac{1}{\hbar} \nabla_k \varepsilon_k \) is the (bare) group velocity of an electron and \( j \) is the current density vector. The conductivity can be determined by taking the zero frequency limit of the imaginary part current-current correlation function, divided by the frequency.

\[
\sigma = \lim_{\omega \to 0} \frac{1}{\omega} \left[ \pi (i\omega \to \omega + i\delta) \right]. \tag{A.4}
\]

The current-current correlation function \( \pi(i\omega_n) \) is given in terms of the \( (D\)-dimensional) volume, \( V_D \), the imaginary time, \( \tau \), with \( \beta = \frac{1}{k_B T} \), \( T_\tau \) the imaginary time-ordering operator and \( \langle ... \rangle \) the expectation value over the system by

\[
\pi_{\alpha\gamma}(i\omega_n) = \frac{-1}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau j_\alpha(\tau) j_\gamma(0) \rangle, \tag{A.5}
\]

which we can then express in the interaction picture as an expansion of the S-matrix

\[
\pi_{\alpha\gamma}(i\omega_n) = \frac{-e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau S(\beta) e^{\tau H_0} j_\alpha(\tau) e^{-\tau H_0} j_\gamma(0) \rangle, \tag{A.6}
\]

\[
\pi_{\alpha\gamma}^{(0)}(i\omega_n) = \pi_{\alpha\gamma}(i\omega_n) - \sum_{n=0}^\infty \pi^{(n)}_{\alpha\gamma}(i\omega_n), \tag{A.7}
\]

Eqn. (A.7) is the lowest order term in the S-matrix expansion, representing non-interacting electrons. As such, the expectation value in Eqn. (A.7) can be rearranged using Wick’s theorem, to obtain [6]

\[
\pi_{\alpha\gamma}^{(0)}(i\omega_n) = \frac{-e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \sum_{p,p',\sigma,\sigma'} v_{p,\alpha} v_{p',\gamma} \langle T_\tau c_{p,\sigma}(\tau) c_{p',\sigma'}(0) c_{p',\sigma'}(0) c_{p,\sigma}(\tau) \rangle. \tag{A.8}
\]
which can then be expressed in terms of the (non-interacting) imaginary time Green’s functions $G^{(0)}(\mathbf{p}, \sigma; \tau) = iT_{c \mathbf{p}, \sigma}(\tau) c_{\mathbf{p}, \sigma}^{\dagger}(0)$, after first imposing the condition that $\mathbf{p} = \mathbf{p}'$ and $\sigma = \sigma'$ (as otherwise the expectation value will vanish), to give

$$
\pi^{(0)}_{\alpha\gamma}(i\omega_n) = \frac{e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \sum_{\mathbf{p}, \sigma} v_{\mathbf{p}, \alpha} v_{\mathbf{p}, \gamma} G^{(0)}(\mathbf{p}, \sigma; \tau) G^{(0)}(\mathbf{p}, \sigma; -\tau)
$$

$$
= \frac{2e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \sum_{\mathbf{p}} v_{\mathbf{p}, \alpha} v_{\mathbf{p}, \gamma} G^{(0)}(\mathbf{p}; \tau) G^{(0)}(\mathbf{p}; -\tau). \tag{A.8}
$$

Eqn. (A.8) is the correlation function for free electrons, and as such, the resistivity derived from it will vanish, as without interactions, there is no mechanism for relaxation. We can include interactions in the expression by substituting the dressed Green’s functions, which account for interactions through scattering via the self-energy,

$$
\pi^{(0)}_{\alpha\gamma}(i\omega_n) = \frac{2e^2}{V_D} \int_0^\beta d\tau e^{i\omega_n \tau} \sum_{\mathbf{p}} v_{\mathbf{p}, \alpha} v_{\mathbf{p}, \gamma} G(\mathbf{p}; \tau) G(\mathbf{p}; -\tau)
$$

$$
= \frac{2e^2}{V_D} \sum_{\mathbf{p}} v_{\mathbf{p}, \alpha} v_{\mathbf{p}, \gamma} \frac{1}{\beta \sum_{\mathbf{ip}_m}} G(\mathbf{p}; \mathbf{ip}_m + i\omega_n) G(\mathbf{p}; \mathbf{ip}_m). \tag{A.9}
$$

In Eqn. (A.9), we have also used the integral to transform the imaginary time Green’s functions into their convolution in the Matsubara formalism, which can later be used to find the real time Green’s functions (in the frequency domain) via analytic continuation. The sum over Matsubara frequencies $i\omega_n$ of products of Green’s functions $S(i\omega_n) \equiv \frac{1}{\beta} \sum_{\mathbf{ip}} G(\mathbf{p}; \mathbf{ip} + i\omega_n) G(\mathbf{p}; \mathbf{ip})$ can be computed in the following way, by first expressing the Green’s functions in the spectral representation ([6] Section 3.5, pp. 136-138),

$$
S(i\omega_n) = \frac{1}{\beta} \sum_{\mathbf{ip}} G(\mathbf{p}; \mathbf{ip} + i\omega_n) G(\mathbf{p}; \mathbf{ip})
$$

$$
= \int \frac{d\varepsilon_1}{2\pi} A(\mathbf{p}, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(\mathbf{p}, \varepsilon_2) \frac{1}{\beta} \sum_{\mathbf{ip}_m} \frac{1}{i\omega_n + \varepsilon_1} \frac{1}{i\omega_n - \varepsilon_2} \tag{A.10}
$$

$$
= \int \frac{d\varepsilon_1}{2\pi} A(\mathbf{p}, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(\mathbf{p}, \varepsilon_2) S_0(i\omega_n), \tag{A.11}
$$

where $S_0(i\omega_n) \equiv \frac{1}{\beta} \sum_{\mathbf{ip}} G^{(0)}(\mathbf{p}; \mathbf{ip} + i\omega_n) G^{(0)}(\mathbf{p}; \mathbf{ip}) = \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{i\omega_n + \varepsilon_2 - \varepsilon_1}$ is computed via a contour integral. Defining the function $f(z)$

$$
f(z) = \frac{1}{iz + i\omega_n - \varepsilon_1} \frac{1}{iz - \varepsilon_2}. \tag{A.12}
$$

We equate the summation as the contour integral as the product of $f(z)$ and the Fermi-Dirac distribution, which generates poles at the desired summation points (the Fermion Matsubara frequencies, given by $p_n = (2n + 1)\pi k_b T$),

$$
I = \lim_{R \to \infty} \int \frac{dz}{2\pi i} f(z) n_f(z)
$$

$$
= \lim_{R \to \infty} \int \frac{dz}{2\pi i} \frac{1}{iz + i\omega_n - \varepsilon_1} \frac{1}{iz - \varepsilon_2} n_f(z),
$$

and choose the contour such that the value of the contour integral to zero,

$$
0 = \sum_i r_i n_f(z_i) + \sum_{\mathbf{ip}_m} f(\mathbf{ip}_m). \tag{A.13}
$$
We can now equate the sum over Matsubara frequencies \( S_0(i\omega_n) \) with the residues of the function \( f(z) \)

\[
S_0(i\omega_n) = \sum_{i\omega_m} f(i\omega_m) = -\sum_{\ell} n_f(\varepsilon_\ell)
\]

\[
= \frac{n_f(\varepsilon_1)}{i\omega_n + \varepsilon_2 - \varepsilon_1} + \frac{n_f(\varepsilon_1 - i\omega_n)}{-i\omega_n + \varepsilon_1 - \varepsilon_2}
\]

\[
= \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{i\omega_n + \varepsilon_2 - \varepsilon_1}.
\]

(A.14)

Thus, the expression for \( S(i\omega_n) \) becomes

\[
S(i\omega_n) = \int \frac{d\varepsilon_1}{2\pi} A(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{i\omega_n + \varepsilon_2 - \varepsilon_1}.
\]

(A.15)

Making the substitution \( i\omega_n = \hbar \omega + i\delta \), we obtain the retarded value,

\[
S(\omega) = \int \frac{d\varepsilon_1}{2\pi} A(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) \left( \frac{n_f(\varepsilon_2) - n_f(\varepsilon_1)}{\hbar \omega + i\delta + \varepsilon_2 - \varepsilon_1} \right)
\]

\[
\text{Im} \{ S(\omega) \} = \int \frac{d\varepsilon_1}{2\pi} A(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) \left( -\pi \frac{(n_f(\varepsilon_2) - n_f(\varepsilon_1)) \delta}{(\hbar \omega + \varepsilon_2 - \varepsilon_1)^2 + \delta^2} \right).
\]

(A.16)

Taking the limit \( \delta \to 0 \) results in a Dirac delta function in the integral,

\[
\lim_{\delta \to 0} \text{Im} \{ S(\omega) \} = -\pi \int \frac{d\varepsilon_1}{2\pi} A(p, \varepsilon_1) \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) (n_f(\varepsilon_2) - n_f(\varepsilon_1)) \delta (\hbar \omega + \varepsilon_2 - \varepsilon_1)
\]

\[
= -\int \frac{d\varepsilon_2}{4\pi} A(p, \varepsilon_2) A(p, \varepsilon_2 + \omega) (n_f(\varepsilon_2) - n_f(\varepsilon_2 + \hbar \omega)),
\]

so, the current-current correlation function is given by

\[
\text{Im} \{ \pi_{\alpha\gamma}^{(0)} (\omega)_R \} = -\frac{e^2}{3m^2v} \sum_p p_\alpha p_\gamma \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) A(p, \varepsilon_2 + \omega) (n_f(\varepsilon_2) - n_f(\varepsilon_2 + \hbar \omega)).
\]

(A.17)

The conductivity is then found by taking the zero frequency limit of the retarded current-current correlation function divided by the frequency \( \omega \),

\[
\sigma_{\alpha\gamma}^{(0)} = \lim_{\omega \to 0} \frac{e^2}{V_D} \sum_p v_\alpha v_\gamma \int \frac{d\varepsilon_2}{2\pi} A(p, \varepsilon_2) A(p, \varepsilon_2 + \omega) \frac{h(n_f(\varepsilon_2) - n_f(\varepsilon_2 + \hbar \omega))}{\hbar \omega}
\]

\[
= e^2 \hbar \int_{2\pi} d^DP \int_{2\pi} A^2(p, \varepsilon) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right)
\]

\[
= e^2 \hbar \int_{2\pi} d^DP \int_{2\pi} A^2(p, \varepsilon) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right).
\]

(A.18)

In the final line of Eqn. (A.18), we have stated the expression for the conductivity in three dimensions, explicitly.

**Expression in terms of the self-energy**

Using the definition of the squared one-band spectral function in the low energy limit given in Eqn. (2.11), we arrive at the expression for the conductivity in terms of the imaginary part of the self-energy \( \Sigma^{\prime\prime}_{k,\omega} \) and wavevector \( k \)

\[
\sigma_{\alpha\gamma}^{(0)} = e^2 \hbar \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} v_{k,\alpha} v_{k,\gamma} \int \frac{d\varepsilon}{2\pi} \left( \Sigma^{\prime\prime}_{k,\omega} (Z\delta (\varepsilon - Z\varepsilon_k)) \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right).
\]

(A.19)
Using the relationship Eqn. (2.58), we investigate the low energy behaviour and find for zero temperature (noting that $\delta (\varepsilon - Z\varepsilon_k)$ can be evaluated at $\varepsilon = Z\varepsilon_F$ and taken outside the energy integral,

\[ \sigma^{(0)}_{\alpha\gamma} = e^2 \hbar \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} v_{k,\alpha} v_{k,\gamma} Z\delta (Z\varepsilon_F - Z\varepsilon_k) \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma'_{k,\omega}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) \]

\[ = e^2 \hbar \int_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^3} v_{k,\alpha} v_{k,\gamma} \delta (\varepsilon_F - \varepsilon_k) \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma'_{k,\omega}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) , \]  

(A.20)

If we consider a diagonal component of the conductivity tensor $\sigma^{(0)}_{xx}$, and assume that $v_{k,x}$ varies slowly at the Fermi surface ($\varepsilon_k = \varepsilon_F$), we can use the definition of the (bare) density of states $D_0(\varepsilon)$ to simplify the expression (A.20) and obtain

\[ \sigma^{(0)}_{xx} (T = 0) = \frac{e^2 \hbar \langle v^2_{k,x} \rangle}{2} \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma'_{k,\omega}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) D_0(\varepsilon_F) \]

\[ = \frac{e^2 \hbar \langle v^2_{k,x} \rangle D_0(\varepsilon_F)}{2} \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma'_{k,\omega}} \right) \left( -\frac{dn_f(\varepsilon)}{d\varepsilon} \right) . \]

(A.21)

**Quadratic Resistivity Coefficient**

Using the relationship Eqn. (2.58), we investigate the low energy behaviour and find for zero temperature (noting that $\frac{dn_f(\varepsilon,T)}{d\varepsilon} \rightarrow \delta (\varepsilon - \varepsilon_F)$ as $T \rightarrow 0$)

\[ \frac{1}{\Sigma'_{k}(T = 0)} = - \left[ \frac{h}{2\tau_0} + \frac{s^2}{\varepsilon_0} \right]^{-1} \]

\[ \sigma^{(0)}_{xx} (T = 0) = \frac{e^2 \hbar \langle v^2_{k,x} \rangle D_0(\varepsilon_F)}{2} \left[ \frac{h}{2\tau_0} \right]^{-1} . \]

(A.22)

Taking the pure limit ($\tau_0 \rightarrow \infty$, $s \rightarrow s_p = \frac{2n}{\pi^2 D_0(\varepsilon_F)}$) the unitarity limit of $s$ [34]), the zero temperature contribution to the resistivity vanishes

\[ \rho_0 = \frac{1}{\sigma^{(0)}_{xx}(T = 0)} = \frac{2s_p}{e^2 \hbar \langle v^2_{k,x} \rangle D_0(\varepsilon_F)} \frac{h}{2\tau_0} \rightarrow 0. \]

(A.23)

For low, but non zero, temperatures

\[ \lim_{\tau_0 \rightarrow 0} \frac{1}{\Sigma'_{k}} = - \lim_{\tau_0 \rightarrow 0} \left[ \frac{h}{2\tau_0} + \frac{s^2 + (\pi k_b T)^2}{\varepsilon_0^2} \right]^{-1} \]

\[ = - \frac{s_p (\varepsilon^2 + (\pi k_b T)^2)}{\varepsilon_0^2} , \]

(A.24)

therefore, the conductivity at low temperatures becomes

\[ \sigma^{(0)}_{xx} (T) = \frac{e^2 \hbar \langle v^2_{k,x} \rangle D_0(\varepsilon_F)}{2} \left[ \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{1}{\Sigma'_{k}} \right) \left( -\frac{dn_f(\varepsilon,T)}{d\varepsilon} \right) \right] \]

\[ = \frac{e^2 \hbar \langle v^2_{k,x} \rangle D_0(\varepsilon_F)}{2} \left[ \int_{-\infty}^{\infty} d\varepsilon \left( -\frac{\varepsilon_0^2}{s_p (\varepsilon^2 + (\pi k_b T)^2)} \right) \left( -\frac{d}{d\varepsilon} \frac{1}{e^{\pi T^2} + 1} \right) \right] . \]

(A.25)
where in the last line of Eqn. (A.24) we have again taken the pure limit \( \tau_0 \to \infty, s \to s_p = \frac{2n}{3\pi D_0(\varepsilon_F)} \). The derivative in Eqn. (A.25) is easily evaluated and simplified via a change of variables \( x = \frac{\varepsilon}{k_B T} \)

\[
\frac{dn_j(\varepsilon, T)}{d\varepsilon} = \frac{-1}{k_B T} \left( e^{\frac{\varepsilon}{k_B T}} + 1 \right)^{-2} e^{\frac{\varepsilon}{k_B T}} = -\frac{1}{k_B T} \frac{e^x}{(e^x + 1)^2} = -\frac{1}{4k_B T} \frac{1}{(e^{x/2} + e^{-x/2})} = -\frac{1}{4k_B T} \text{sech}^2 \left( \frac{x}{2} \right),
\]

\[
\frac{1}{\Sigma_k'} = -\frac{x_0^2}{s_p (x^2 + \pi^2)}.
\]  

Now, we can evaluate Eqn. (A.25)

\[
\sigma_{xx}^{(0)}(T) = \frac{e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F)}{8} \left[ \int_{-\infty}^{\infty} dx \left( \frac{x_0^2}{s_p (x^2 + \pi^2)} \right) \left( \text{sech}^2 \left( \frac{x}{2} \right) \right) \right]
\]

\[
= \frac{e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F) \varepsilon_0^2}{2s_p} \left[ \frac{1}{4k_B T^2} \int_{-\infty}^{\infty} dx \left( \text{sech}^2 \left( \frac{x}{2} \right) \right) \right].
\]  

Performing the integral in Eqn.(A.28) obtains a value of \( \int_{-\infty}^{\infty} dx \left( \frac{\text{sech}^2 \left( \frac{x}{2} \right)}{x^2 + \pi^2} \right) \) = \( \frac{1}{3} \) (see Appendix A.3.1), which leads to a value for the A coefficient of

\[
A = \frac{1}{T^2} \left( \frac{e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F) \varepsilon_0^2}{2s_p} \right) \left[ \frac{1}{12k_B T^2} \right]^{-1}
\]

\[
= \frac{24s_p k_B^2}{e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F) \varepsilon_0^2}.
\]  

Making the substitution \( s_p = \frac{2n}{3\pi D_0(\varepsilon_F)} \), we arrive at the final expression for the A coefficient

\[
A = \frac{16n k_B^2}{\pi e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F) \varepsilon_0^2} = \frac{16nk_B^2}{\pi e^2 \hbar \langle v_{k,x}^2 \rangle D_0(\varepsilon_F) \varepsilon_0^2}.
\]  

### A.1.2 Heat Capacity

The heat capacity for a one band material can be found easily, by taking the derivative of Eqn. (2.69) with respect to energy and substituting the value into the heat capacity expression Eqn. (1.2), to obtain

\[
C_{el}(T) = \gamma T
\]

\[
= \pi^2 k_B^2 D_0(\varepsilon_F) \left( 1 - \frac{\partial \Sigma'}{\partial \varepsilon} \right) T
\]

\[
= \frac{\pi^2 k_B^2 D_0(\varepsilon_F)}{3} \left( 1 + \frac{2s_p}{\pi \varepsilon_0} (1 + \xi) \right) T.
\]  

If we assume that \( s_p \gg \varepsilon_0 \), we arrive at an expression for \( \gamma \), with \( s_p = \frac{2n}{3\pi D_0(\varepsilon_F)} \)

\[
\gamma = \frac{4nk_B^2 (1 + \xi)}{9\varepsilon_0}.
\]
A.1.3 The Kadowaki-Woods Ratio

For a one band system, we have the relationships (A.30) and (A.32)

\[
A_i = \frac{16nk_b^2}{\pi e^2h(v_F^2)D_0^2(\varepsilon_F)\varepsilon_0^2},
\]

\[
\gamma = \frac{4nk_b^2(1 + \xi)}{9\varepsilon_0},
\]

and the Kadowaki-Woods ratio for a one band system is

\[
R_{KW} = \frac{A}{\gamma^2}
\]

\[
= \frac{16nk_b^2}{\pi e^2h(v_F^2)D_0^2(\varepsilon_F)\varepsilon_0^2} \left( \frac{4nk_b^2(1 + \xi)}{9\varepsilon_0} \right)^{-2}
\]

\[
= \frac{16nk_b^2}{\pi e^2h(v_F^2)D_0^2(\varepsilon_F)\varepsilon_0^2} \frac{81\varepsilon_0^2}{16n^2k_b^4(1 + \xi)^2}
\]

\[
= \frac{81}{4\pi e^2h(v_F^2)D_0^2(\varepsilon_F)n k_b^2}.
\]

(A.33)

In the last line of Eqn. (A.33), we have used the upper limit of \( \xi \) (\( \xi = 1 \)) to find the maximum of the Kadowaki-Woods ratio. Following [20], we now take the material-dependent parameters out of the expression to obtain the more universal ratio,

\[
\frac{A}{\gamma^2}f_{dx}(n) = \frac{81}{4\pi e^2n k_b^2},
\]

(A.34)

where we have defined the material-dependent function \( f_{dx}(n) = \langle v_F^2 \rangle D_0^2(\varepsilon_F)n \), where all values are given by the non-interacting system.

A.2 Non-zero interband self energy in the two band model

If we avoid making the approximation that the interband elements of the self-energy are vanishingly small, we have the expression for the intraband spectral density functions Eqns. (2.26), which can be rearranged to yield the expression, for \( b \neq a \)

\[
A_{k,\varepsilon;a,a} = \frac{-2\eta_{k;b,b}}{\eta_{k;a,a} - \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2} \left[ \Gamma_{k;a,a} + \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \Gamma_{k,b,b} \right]
\]

\[
\phantom{A_{k,\varepsilon;a,a}} = \frac{-2\eta_{k;a,a} - \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \eta_{k,b,b}}{\left[ \eta_{k;a,a} - \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \eta_{k,b,b} \right]^2 + \left[ \Gamma_{k;a,a} + \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \Gamma_{k,b,b} \right]^2}.
\]

(A.35)

If we again take the low energy limit, we obtain the expressions for the spectral density function and spectral density function squared

\[
\lim_{\Gamma \to 0} A_{k,\varepsilon;a,a} = -2\pi\delta \left( \eta_{k;a,a} - \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \eta_{k;b,b} \right),
\]

(A.36)

\[
\lim_{\Gamma \to 0} A_{k,\varepsilon;a,a}^2 = \frac{-2\pi\delta \left( \eta_{k;a,a} - \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \eta_{k;b,b} \right)}{\left[ \Gamma_{k;a,a} + \left( \frac{\Sigma_{k,a,b}^{\prime}}{\eta_{k,b,b}} \right)^2 \Gamma_{k,b,b} \right]},
\]

(A.37)
The two band conductivity is then
\[\sigma_{xx}^{(0)} = \hbar e^2 \int \frac{d^3k}{(2\pi)^3} |v_{k,x}|^2 \int \frac{d\varepsilon}{(2\pi)} \sum_a A_{a,a}^2 (p, \varepsilon) \left(-\frac{dn_f(\varepsilon)}{d\varepsilon}\right)\]

\[= \hbar e^2 \int \frac{d^3k}{(2\pi)^3} |v_{k,x}|^2 \int \frac{d\varepsilon}{(2\pi)} \left[ \frac{\delta \left( \eta_{k;1,1} - \left(\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right)^2 \eta_{k;2,2} \right)}{\Gamma_{k;1,1} + \left(\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right)^2 \Gamma_{k;2,2}} + \frac{\delta \left( \eta_{k;2,1} - \left(\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right)^2 \eta_{k;1,1} \right)}{\Gamma_{k;2,1} + \left(\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right)^2 \Gamma_{k;2,2}} \right] \left(-\frac{dn_f(\varepsilon)}{d\varepsilon}\right)\]  
(A.38)

which can be seen to approach the form of Eqn. (2.54) for \(\left|\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right| \ll 1\), and, in the opposite limit \(\left|\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right| \gg 1\) the corresponding delta function takes the form \(\delta \left( \left(\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right)^2 \eta_{k;1,1} \right)\) and it is obvious that argument of the delta function will never be zero in this limit, and there will be no contribution to the conductivity from the \(a\) band. This is reasonable, considering that the limit is equivalent to assuming that the magnitude of the scattering potential is much larger than the difference between the energy and the Fermi energy, \(\eta_{k;a,a} = \varepsilon_F - \varepsilon_{k;a,a}\), so that the scattering is significant enough to reduce the conductivity. The intermediate range is more complicated. For example, if \(\left|\frac{\sum_{\eta_{k;1,2}}}{\eta_{k;1,2}}\right| = 1\) we arrive at an expression for the conductivity

\[\sigma_{xx}^{(0)} = \hbar e^2 \int \frac{d^3k}{(2\pi)^3} |v_{k,x}|^2 \int \frac{d\varepsilon}{(2\pi)} \left[ -\frac{2\delta (\eta_{k;1,1} - \eta_{k;2,2})}{\Gamma_{k;1,1} + \Gamma_{k;2,2}} \right] \left(-\frac{dn_f(\varepsilon)}{d\varepsilon}\right)\]  
(A.39)

and the conductivity will be zero if there is a band gap, and non zero in gapless materials.

### A.3 Integrals and Special Relations

#### A.3.1 \(\int_{-\infty}^{\infty} dx \frac{\text{sech}^2 \left(\frac{x}{\beta}\right)}{x^2 + \pi^2}\)

We define the integral [68]

\[I = \int_{-\infty}^{\infty} dx \frac{\text{sech}^2 \left(\frac{x}{\beta}\right)}{x^2 + \pi^2} = \frac{1}{\pi^2} \int_{-\infty}^{\infty} dx \frac{x^2 + \pi^2 - x^2}{x^2 + \pi^2} \text{sech}^2 \left(\frac{x}{2}\right)\]

\[= \frac{1}{\pi^2} \int_{-\infty}^{\infty} dx \text{sech}^2 \left(\frac{x}{2}\right) - \frac{2}{\pi^2} \int_{0}^{\infty} dx \frac{x^2}{x^2 + \pi^2} \text{sech}^2 \left(\frac{x}{2}\right)\]

\[= \frac{1}{\pi^2} \left[ 2\tanh \left(\frac{x}{2}\right) \right]_{-\infty}^{\infty} - \frac{8}{\pi^2} \int_{0}^{\infty} dx \frac{x^2}{x^2 + \pi^2} \frac{e^x}{(1 + e^x)^2}\]

\[= \frac{4}{\pi^2} \left[ 1 - 2 \int_{0}^{\infty} dx \frac{x^2}{x^2 + \pi^2} \frac{e^x}{(1 + e^x)^2} \right]\]

\[= \frac{4}{\pi^2} \left[ 1 + 2 \frac{\partial}{\partial \alpha} \left[ \int_{0}^{\infty} dx \frac{x}{x^2 + \pi^2} \frac{1}{(1 + e^{\alpha x})} \right]_{\alpha=1} \right].\]  
(A.40)

From [63],

\[\int_{0}^{\infty} dx \frac{x}{x^2 + \beta^2 (1 + e^{\alpha x})} = \frac{1}{2} \left[ \psi \left( \frac{\beta \nu}{2} + \frac{1}{2} \right) - \ln \left( \frac{\beta \nu}{2\pi} \right) \right],\]  
(A.41)
where $\psi(x)$ is the digamma function. With $\beta = \pi$ and $\mu = \alpha$

\[
I = \frac{4}{\pi^2} \left[ 1 + \frac{\partial}{\partial \alpha} \left( \psi \left( \frac{\alpha}{2} + \frac{1}{2} \right) - \ln \left( \frac{\alpha}{2} \right) \right)_{\alpha=1} \right] \\
= \frac{4}{\pi^2} \left[ 1 + \frac{1}{2} \psi' (1) - 1 \right] \\
= \frac{2}{\pi^2} \psi' (1).
\] (A.42)

Again from [63]

\[
\psi' (1) = \frac{\pi^2}{6},
\] (A.43)

so,

\[
I = \frac{2}{\pi^2} \frac{\pi^2}{6} = \frac{1}{3},
\] (A.44)

as expected from numerical calculations.

### A.3.2 Eqn. (4.12)

We have, from momentum and energy conservation, Eqn. (4.10),

\[
p'^2_1 = \frac{p'_1 p_2 \sin (\phi_2)}{\cos (u)} \sin (\phi'_1 + u) - p_1 p_2 \cos (\phi_2)
\]

\[
p'^2_1 p_2^2 \sin^2 (\phi_2) \cos^2 (u) \sin^2 (\phi'_1 + u) = p'^4_1 + 2p'^2_1 p_1 p_2 \cos (\phi_2) + p'^2_1 p_2^2 \cos^2 (\phi_2),
\] (A.45)

and the derivative, Eqn. (4.11)

\[
\left| \frac{dp'^2_1}{d\phi'_1} \right|_{\phi'_1 = \phi_0} = \left[ 4p'^2_1 p_2^2 \sin^2 (\phi_2) \cos^2 (\phi'_1 + u) \right]^{1/2}.
\] (A.46)

We first combine the two using the trigonometric identity,

\[
4p'^2_1 p_2^2 \frac{\sin^2 (\phi_2) \cos^2 (\phi'_1 + u)}{\cos^2 (u)} = 4p'^2_1 p_2^2 \frac{\sin^2 (\phi_2)}{\cos^2 (u)} \left[ 1 - \sin^2 (\phi'_1 + u) \right]
\]=

\[
4p'^2_1 p_2^2 \frac{\sin^2 (\phi_2)}{\cos^2 (u)} - 4 \left( p'^4_1 + 2p'^2_1 p_1 p_2 \cos (\phi_2) + p'^2_1 p_2^2 \cos^2 (\phi_2) \right),
\] (A.47)

and make use of the definitions of the arctangent and cosine functions, [63]

\[
arctan (x) = \frac{i}{2} \log (1 - ix) - \log (1 + ix),
\]

\[
\cos (x) = \frac{1}{2} \left( e^{ix} + e^{-ix} \right),
\]

\[
\cos (\arctan (x)) = \frac{1}{2} \left( e^{- \left[ \log(1-ix)^{\frac{1}{2}} - \log(1+ix)^{\frac{1}{2}} \right]} + e^{- \left[ \log(1-ix)^{\frac{1}{2}} - \log(1+ix)^{\frac{1}{2}} \right]} \right),
\]

\[
= \left( \frac{(1 + ix)^{\frac{1}{2}}}{(1 - ix)^{\frac{1}{2}}} + \frac{(1 - ix)^{\frac{1}{2}}}{(1 + ix)^{\frac{1}{2}}} \right)
= \left( \frac{(1 - ix)(1 + ix)^{\frac{1}{2}}}{(1 + ix)(1 - ix)^{\frac{1}{2}}} \right) = \left[ 1 + x^2 \right]^{\frac{1}{4}},
\] (A.48)
to calculate $\cos^2(u) = \left[ 1 + \left( \frac{p_1 + p_2 \cos(\phi_2)}{p_2^2 \sin^2 \phi_2} \right)^2 \right]^{-1}$ and make the simplification

$$4p_1^2 p_2^2 \frac{\sin^2 (\phi_2)}{\cos^2 (u)} \cos^2 (\phi_1 + u) = 4p_1^2 p_2^2 \left[ \frac{1 + (p_1 + p_2 \cos(\phi_2))^2}{p_2^2 \sin^2 \phi_2} \right] - 4p_1^4 - 8p_1^2 p_2 \cos(\phi_2) - 4p_1^2 p_2^2 \cos^2(\phi_2)$$

$$= 4p_1^2 \left( p_1^2 + p_2^2 + 2p_1 p_2 \cos(\phi_2) \right) - 4p_1^4 - 8p_1^2 p_2 \cos(\phi_2) - 4p_1^2 p_2^2 \cos^2(\phi_2)$$

$$= 4p_1^2 \left( p_1^2 + p_2^2 - p_1^2 \right) - 4p_1^2 p_2^2 \cos^2(\phi_2)$$

$$\left| \frac{dp_2^2}{d\phi_1} \right|_{\phi_1 = \phi_0} = \left[ 4p_1^2 \left( p_1^2 + p_2^2 + p_1^2 \right) - 4p_1^2 p_2^2 \cos^2(\phi_2) \right]^{1/2}.$$  

**Graphene**

For the case of graphene, we have the similar relationship

$$\cos^2(-v) = \cos^2 \left( \arctan \left( \frac{-p_1 + p_1' \cos \phi'}{p_1' \sin \phi'} \right) \right) = \left[ 1 + \left( \frac{-p_1 + p_1' \cos \phi'}{p_1' \sin \phi'} \right)^2 \right]^{-1} = \frac{p_1'^2 \sin^2 \phi'}{p_1'^2 \sin^2 \phi' + p_1'^2 - 2p_1 p_1' \cos \phi' + p_1'^2 \cos^2 \phi'} = \frac{p_1'^2 \sin^2 \phi'}{p_1'^2 + p_1'^2 - 2p_1 p_1' \cos \phi'},$$

(A.49)
BIBLIOGRAPHY


