Diffusion of Dirac fermions across a topological merging transition in two dimensions

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A continuous deformation of a Hamiltonian possessing at low energy two Dirac points of opposite chiralities can lead to a gap opening by merging of the two Dirac points. In two dimensions, the critical Hamiltonian possesses a semi-Dirac spectrum: linear in one direction but quadratic in the other. We study the transport properties across such a transition, from a Dirac semi-metal through a semi-Dirac phase towards a gapped phase. Using both a Boltzmann approach and a diagrammatic Kubo approach, we describe the conductivity tensor within the diffusive regime. In particular, we show that both the anisotropy of the Fermi surface and the Dirac nature of the eigenstates combine to give rise to anisotropic transport times, manifesting themselves through an unusual matrix self-energy.

I. INTRODUCTION

The discovery of graphene has triggered a lot of work on the exotic transport properties of Dirac-like particles in solids1. Indeed, the graphene electronic spectrum is made of two sub-bands which touch at two inequivalent points in reciprocal space. Near the touching points, named Dirac points, the spectrum has a linear shape and the electron dynamics is well described by a 2D Dirac equation for massless particles. Due to the structure of the honeycomb lattice, the wave functions have two components corresponding to the two inequivalent sites of the lattice, and the Hamiltonian is a $2 \times 2$ matrix. To describe the low energy properties, the original Hamiltonian is replaced by two copies of a 2D Dirac equation

$$H = \pm c \vec{p} \cdot \vec{\sigma}$$

where the velocity $c \simeq 10^5$ m.s$^{-1}$. This linearization is possible because the energy of the saddle point separating the two Dirac cones (valleys) is very large ($\approx 3$ eV) compared to the Fermi energy and temperature scales. Other realizations of Dirac-like physics in two dimensions have been proposed in the organic conductor (BEDT-TTF)$_2$I$_3$ under pressure2-5, and has been observed in artificially assembled nanostructures6-10 and ultracold atoms11,12. Besides these two dimensional realizations, the existence and properties of semi-metallic phases in three dimensions have recently been studied13,14.

To go beyond and in order to account for a structure which consists in two Dirac points separated by a saddle point, one needs an appropriate low energy $2 \times 2$ Hamiltonian. Moreover, such a description is mandatory in situations where, by varying band parameters, the Dirac points can be moved in reciprocal space. Since these Dirac points are characterized by opposite topological charges, they can even annihilate each other15-19. This merging is therefore a topological transition. It has been shown that, at the transition, the electronic dispersion is quite unusual since it is quadratic in one direction and linear in the other direction (the direction of merging). This ”semi-Dirac”20 spectrum has new properties intermediate between a Schrödinger and a Dirac spectrum. The vicinity of the topological transition can be described by the following Hamiltonian in two dimensions18,19:

$$H = \left( \Delta + p_x^2 \right) \sigma_x + c_y p_y \sigma_y \cdot$$

It has been coined ”Universal Hamiltonian” since the merging scenario of two Dirac points related by time reversal symmetry is uniquely described by this Hamiltonian18,19. The parameter $\Delta$ drives the transition ($\Delta = 0$) between a semi-metallic phase ($\Delta < 0$) with two Dirac points and a gapped phase ($\Delta > 0$), see Figs. 1,2.

The evolution of several thermodynamic quantities like the specific heat and the Landau level spectrum has been studied in details18,19.

Figure 1. This work addresses the transport properties for an electronic spectrum undergoing a topological merging transition as depicted in this figure, and commented in more details in Fig. 2.

In this paper we address the evolution of the conductivity tensor across the merging transition (Figs. 1,2). A first objective of this work is to characterize the transport properties as a possible signature of the evolution of
the underlying band structure. On a more fundamental perspective, an additional interest of this problem stands from two important ingredients in the description of diffusive transport. First, at low energy the electronic wave functions have a spinorial structure which leads to effective anisotropic scattering matrix elements (similar to the case of a scalar problem with anisotropic scattering due to a disorder potential with finite range). This leads to a transport scattering time $\tau^{\text{tr}}$ different from the elastic scattering time $\tau_e$, as in graphene for point-like impurities where $\tau^{\text{tr}} = 2\tau_e$. Second, the anisotropy of the dispersion relation leads to an additional complexity: the scattering times become themselves anisotropic and depend on the direction of the applied electric field. We show that within the Green’s function formalism this anisotropy manifests itself into a rather unusual matrix structure of the self-energy. A comparison between a Boltzmann approach and a perturbative Green’s function formalism allows for a detailed understanding of this physics.

The outline of the paper is the following. In the next section, we recall the model, i.e. the Universal Hamiltonian with coupling to impurities described by a point-like white noise potential. We define a directional density of states and derive the angular dependence of the elastic scattering time. In section III, we use the Boltzmann equation to calculate the conductivity tensor. As a result of the two important ingredients mentioned above, the conductivity along a direction $\alpha$ is not simply proportional to the angular averaged squared velocity $\langle v^2_\alpha(\theta) \rangle$ because: (i) the elastic scattering time has also an angular dependence due to the elastic anisotropy of the spectrum, so that one should consider the average $\langle v^2_\alpha(\theta) \tau_e(\theta) \rangle$: (ii) since the matrix elements of the interaction get an angular dependence, it will lead to transport times different of the elastic time. These transport times depend on the direction $\alpha$ and, to obtain the conductivity, we will have to consider the average $\langle v^2_\alpha(\theta) \tau^{\text{tr}}(\theta) \rangle$. These results obtained from Boltzmann equation are confirmed by a diagrammatic calculation presented in section IV. We discuss our results in the last section.

II. THE MODEL

A. Hamiltonian and Fermi surface parametrization

We consider the model described by the Hamiltonian

$$H = H^0 + V,$$

(3)

where the disorder potential $V$ is defined and discussed in section II C and the Hamiltonian for the pure system is defined as

$$H^0 = \left[ \Delta + \frac{p_x^2}{2m} \right] \sigma_x + c_y p_y \sigma_y.$$ 

(4)

In the present and the following sections (II A and II B) we start by discussing a few properties of the Hamiltonian $H^0$ without disorder. For $\Delta > 0$ this Hamiltonian describes a gapped phase. When $\Delta < 0$, it describes two Dirac cones with opposite chiralities, hereafter named a Dirac phase. Note that these Dirac cones are in general anisotropic with respective velocities in the $x$ and $y$ directions $c_x = \sqrt{2}|\Delta|/m$ and $c_y$. The energy spectrum is given by

$$\epsilon^2 = \left( \frac{p_x^2}{2m} + \Delta \right)^2 + (c_y p_y)^2.$$ 

(5)

We will consider only the case of positive energies $\epsilon > 0$, as the situation $\epsilon < 0$ can be deduced from particle-hole symmetry. Fig. 2 presents the different regimes discussed in this paper.

Parametrization of the constant energy contours of Eq. (5) is done by taking advantage of the $p_x$ parity. For each half plane $p_x \leq 0$ we use the parametrization

$$\frac{p_x^2}{2m} + \Delta = \epsilon \cos \theta ; \quad c_y p_y = \epsilon \sin \theta ; \quad \eta_p = \text{sign}(p_x) = \pm 1,$$

(6)

where $\theta \in [-\theta_0, \theta_0]$ is a coordinate along the constant energy contour. Its range depends on the topology of the constant energy contour, and thus on the energy $\epsilon$, see Fig. 3. Specifying the discussion to the Fermi surface associated with the Fermi energy $\epsilon_F$, we can distinguish two cases:

(i) Low energy metal with two disconnected Fermi surfaces when $\Delta < 0$ and $\epsilon_F < -\Delta$. In this case $\theta_0 = \pi$. This corresponds to the energy spectrum (a) of Fig. 2.

(ii) High energy metal with a single connected Fermi surface for $\epsilon_F > |\Delta|$. In this case $\cos \theta_0 = \Delta/\epsilon_F$. For $\Delta < 0$, $\theta_0$ varies from $\pi$ for $\epsilon_F = -\Delta$ to $\pi/2$ for $\epsilon_F \gg -\Delta$. For $\Delta > 0$, $\theta_0$ varies from $\pi/2$ for $\epsilon_F \gg \Delta$ to $\pi$ for $\epsilon_F \rightarrow \Delta$. This corresponds to the energy spectra (b), (c) of Fig. 2.

The eigenstates of positive energy corresponds to wave
functions conveniently expressed with the parametrization of the constant energy contour

\[ \psi_\mathbf{k}(\mathbf{r}) = \frac{1}{\sqrt{2L}} \left( \frac{1}{e^{i\eta_\mathbf{k}}} \right) e^{i\mathbf{k}\cdot\mathbf{r}} , \]  

(7)

where \( \eta_\mathbf{k} \) is defined by inversion of Eq. (6), and \( \mathbf{p} = \hbar \mathbf{k} \).

From now on, we will set \( L = 1 \). The group velocity varies along the constant energy contour according to:

\[ v_x(\eta_\mathbf{p}, \theta) = \eta_\mathbf{p} \sqrt{\frac{2\epsilon}{m}} \cos \theta \sqrt{\cos \theta - \delta} , \]  

(8a)

\[ v_y(\eta_\mathbf{p}, \theta) = c_y \sin \theta , \]  

(8b)

where throughout this paper we use the reduced parameter \( \delta = \Delta/\epsilon \). The evolution of the velocity along constant energy contours is shown on Fig. 4.

B. Density of States

We define a directional density of states along the constant energy contour parametrized by \( \theta \) from the equality

\[ \int \frac{dp_x dp_y}{(2\pi \hbar)^2} = \int \frac{dk_x dk_y}{(2\pi)^2} = \int \rho(\epsilon, \theta) \, d\epsilon \, d\theta \]  

(9)

with

\[ \rho(\epsilon, \theta) = \frac{\sqrt{2m\epsilon}}{(2\pi \hbar)^2 c_y} \frac{1}{2\sqrt{\cos \theta - \delta}} . \]  

(10)

The density of states is then obtained by the integral

\[ \rho(\epsilon) = 2 \int_{-\theta_0}^{\theta_0} d\theta \rho(\epsilon, \theta) \]  

(11)

where the extra factor 2 accounts for the sign of \( p_x \). The integral gives

\[ \rho(\epsilon) = \frac{\sqrt{2m\epsilon}}{(2\pi \hbar)^2 c_y} I_1(\delta) , \]  

(12)

with the function

\[ I_1(\delta) = \int_{-\theta_0}^{\theta_0} \frac{d\theta}{\sqrt{\cos \theta - \delta}} , \]  

(13)

where \( \theta_0 = \arccos(\delta) \) when \( |\delta| < 1 \) and \( \theta_0 = \pi \) otherwise. From Eqs. (10,12), we can rewrite \( \rho(\epsilon, \theta) \) as

\[ \rho(\epsilon, \theta) = \frac{\rho(\epsilon)}{2 I_1(\delta) \sqrt{\cos \theta - \delta}} . \]  

(14)
C. Disorder Potential and Elastic Scattering Time

The disorder part \( V \) of the Hamiltonian accounts for the inhomogeneities in the system. This random potential \( V(\vec{r}) \) is assumed to describe a gaussian point-like uncorrelated disorder, characterized by two cumulants

\[
\overline{V(\vec{r})} = 0, \quad \overline{V(\vec{r})V(\vec{r}')} = \gamma \delta(\vec{r} - \vec{r}').
\]

where the overline denotes a statistical average over realizations of the random potential. The presence of this random potential induces a finite lifetime for the eigenstates of momentum \( \vec{k} \) of the pure model (4), called elastic scattering time, and obtained from the Fermi golden rule:

\[
\frac{\hbar}{\tau_e(\vec{k})} = 2\pi \int \frac{d^2k'}{(2\pi)^2} \delta(\epsilon' - \epsilon) |\mathcal{A}(\vec{k}, \vec{k}')|^2 ,
\]

where the scattering amplitude is defined by

\[
\mathcal{A}(\vec{k}, \vec{k}') = \langle \psi_{\vec{k}'} | V | \psi_{\vec{k}} \rangle .
\]

For uncorrelated point-like disorder, the angular dependence of this scattering amplitude originates from the eigenstates overlap and one has

\[
|\mathcal{A}(\vec{k}, \vec{k}')|^2 = \frac{\gamma}{2} \left( 1 + \cos(\theta_{\vec{k}} - \theta_{\vec{k}'}) \right) .
\]

Defining \( \tau_e(\epsilon, \theta) = \tau_e(\vec{k}) \) where \( \epsilon, \theta \) and \( \vec{k} \) are related through Eq. (6), we can express the elastic scattering time as an integral

\[
\frac{\hbar}{\tau_e(\epsilon, \theta)} = 2\pi \gamma \int_{-\theta_0}^{\theta_0} d\theta' \rho(\epsilon, \theta') \left[ 1 + \cos(\theta - \theta') \right] .
\]

Introducing the bare scattering time

\[
\tau_e^0(\epsilon) = \frac{\hbar}{\pi \gamma \rho(\epsilon)} ,
\]

we can rewrite (19) in the form

\[
\tau_e(\epsilon, \theta) = \frac{\tau_e^0(\epsilon)}{1 + r(\delta) \cos \theta} ,
\]

where the density of states \( \rho(\epsilon) \) is given by (12). The denominator of this expression exactly accounts for the anisotropy of the scattering time. As a convenient parametrization of this property, we have introduced the anisotropy function \( r(\delta) \) which will be used throughout this paper:

\[
r(\delta) = J_1(\delta) / I_1(\delta) ,
\]

with the function \( I_1(\delta) \) defined in (13) and

\[
J_1(\delta) = \int_{-\theta_0}^{\theta_0} \frac{d\theta \cos \theta}{\sqrt{\cos \theta - \delta}} ,
\]

Figure 5. Function \( r(\delta) \) parametrizing the angular dependence of the elastic scattering time \( \tau_e \) plotted as a function of \( \delta = \Delta/\epsilon \). It has the limits \( r(\delta \to -\infty) \approx 1/(4\delta) \), \( r(-1) = -1 \), \( r(0) = 2\Gamma(3/4)^4/\pi^2 \approx 0.456947 \), \( r(1) = 1 \). In this figure, as in following figures, we systematically reserve the colors: blue for the Dirac phase \( \delta < 0 \), black for the gapped phase \( \Delta > 0 \) and red for the semi-Dirac point.

where \( \theta_0 = \arccos(\delta) \) when \( |\delta| < 1 \) and \( \theta_0 = \pi \) otherwise. The function \( r(\delta) \) is plotted in Fig. 5. Deep in the Dirac phase \( \Delta < 0 \), at low energy \( \epsilon \ll |\Delta| \), one has

\[
r(\delta) \to \frac{1}{4|\delta|} = -\frac{\epsilon}{4|\Delta|} \ll 1 ,
\]

so that the anisotropy can be neglected in Eq. (21) and we recover a scattering time independent of the direction of propagation as standard for Dirac fermions.

III. DIFFUSIVE REGIME FROM THE BOLTZMANN EQUATION

We now consider the transport properties of the model (3) at a fixed energy \( \epsilon \) large enough so that the condition \( k l_e \gg 1 \) is fulfilled, \( l_e \) being a typical elastic mean free path. Therefore we will not consider the close vicinity of a Dirac point and the associated physics of minimal conductivity\(^{21,22}\). For a system of typical size much larger than this mean free path \( l_e \), this corresponds to the regime of classical diffusion. We describe this regime first with a standard Boltzmann equation, before turning to a complementary but equivalent diagrammatic approach based on Kubo formula for the conductivity. The use of these two approaches will reveal the physics hidden between the technical specificities of the diffusive transport for the model we consider.
A. Boltzmann equation

We start from the Boltzmann equation\(^{23,24}\) expressing the evolution of the distribution function \(f(\vec{k}, \vec{r})\):

\[
\frac{df}{dt} + \frac{d\vec{r}}{dt} \nabla f + \frac{d\vec{k}}{dt} \nabla_k f = I[f] , \tag{25}
\]

where \(I[f]\) is the collision integral defined below. The position \(\vec{r}\) and momentum \(\vec{k}\) parametrizing the distribution function \(f(\vec{k}, \vec{r})\) are classical variables, whose time evolutions entering Eq.\,(25) are described by the semi-classical equations\(^{25,26}\)

\[
\frac{d\vec{r}}{dt} = \vec{v}(\vec{k}) + \frac{d\vec{k}}{dt} \times \vec{F}_k \tag{26}
\]

\[
\hbar \frac{d\vec{k}}{dt} = -e\vec{E} - e\frac{d\vec{r}}{dt} \times \vec{B} \tag{27}
\]

with the group velocity \(\vec{v}(\vec{k}) = \hbar^{-1}(\partial \epsilon(\vec{k})/\partial \vec{k})\), \(\vec{B}\) is a local magnetic field, and \(\vec{F}_k = i\nabla \times (\psi \nabla \psi^* \vec{k})\) is the Berry curvature. In the present case, we consider the response of the distribution function \(f(\vec{k}, \vec{r})\) due to a uniform weak electric field \(\vec{E}\): we can neglect the gradient \(\nabla \vec{r} f\) in Eq.\,(25) and drop the spatial dependence of \(f\). Due to the absence of magnetic field, we deduce from Eqs.\,(25,27) that a stationary out-of-equilibrium distribution \(f(\vec{k})\) satisfies the simpler equation

\[
-\frac{e}{\hbar} \vec{E} \cdot \nabla_k f = I[f] . \tag{28}
\]

where \(f\) is now as function of \(\vec{k}\) and the collision integral is expressed as

\[
I[f] = 2\pi \int d^2\vec{k}' \frac{d^2\vec{k}'}{(2\pi)^2} \delta(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}) |A(\vec{k}, \vec{k}')|^2 \left( f(\vec{k}') - f(\vec{k}) \right) . \tag{29}
\]

By assuming the perturbation to be weak, we can expand the stationary out-of-equilibrium distribution \(f(\vec{k})\) around the equilibrium Fermi distribution \(f^0(\vec{k}) = n_F(\epsilon_{\vec{k}})\) following the ansatz\(^{23,24}\)

\[
f(\vec{k}) = f^0(\vec{k}) + e \frac{\partial n_F}{\partial \epsilon} \vec{A}(\vec{k}) \cdot \vec{E} , \tag{30}
\]

where the vector \(\vec{A}\) has the dimension of a length, and its components correspond to transport lengths in the different spatial directions. They are related to transport times through the definition \(\Lambda_\alpha(\vec{k}) = v_\alpha(\vec{k}) \tau^\alpha(\vec{k})\). Eq.\,(30) can be rewritten as a shift of energies by the field:

\[
f(\vec{k}) = n_F(\epsilon_{\vec{k}} + e \vec{A}(\vec{k}) \cdot \vec{E}) . \tag{31}
\]

In the case of an isotropic Fermi surface, we do not expect this shift to depend on the direction of application of the field \(\vec{E}\): in that case a unique transport time \(\tau^\alpha\) is necessary to describe the stationary distribution\(^{24}\). Here, for an anisotropic Fermi surface such as (5), we generically expect the response of the distribution function to depend on the direction of the electric field \(\vec{E}\)\(^{27-29}\). For an electric field applied in the \(x\) or \(y\) direction, this leads to the definition of different anisotropic transport times \(\tau^\alpha_x, \tau^\alpha_y\). From Eqs.\,(28,29,30), one obtains

\[
\vec{v}(\vec{k}) = \frac{1}{\hbar} \left. \frac{\partial \epsilon}{\partial \vec{k}} \right|_{\epsilon = \epsilon_{\vec{k}}} = 2\pi \int d^2\vec{k}' \frac{d^2\vec{k}'}{(2\pi)^2} \delta(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}) |A(\vec{k}, \vec{k}')|^2 \left( \vec{A}(\vec{k}') - \vec{A}(\vec{k}) \right) , \tag{31}
\]

By using the parametrization (6) on the contour of constant energy \(\epsilon\), each component \(\alpha\) of the velocity obeys the equation (to lighten notation, we omit the energy \(\epsilon\) in the argument of the quantities in the next expressions):

\[
v_\alpha(\eta_p, \theta) = \frac{\Lambda_\alpha(\eta_p, \theta)}{\tau_\epsilon(\theta)} - \frac{\pi \gamma}{\hbar} \sum_{\eta_p'} \int_{-\theta_0}^{\theta_0} d\theta' \rho(\theta') [1 + \cos(\theta - \theta')] \Lambda_\alpha(\eta_p', \theta') . \tag{32}
\]

The transport times \(\tau^\alpha_\epsilon(\epsilon, \theta)\) are defined as

\[
\Lambda_\alpha(\epsilon, \eta_p, \theta) = v_\alpha(\epsilon, \eta_p, \theta) \tau^\alpha_\epsilon(\epsilon, \theta) . \tag{33}
\]

We now assume the following ansatz, namely that the transport times and the elastic scattering time have the same angular dependence:

\[
\tau^\alpha_\epsilon(\epsilon, \theta) = \lambda_\epsilon(\epsilon) \tau_\epsilon(\epsilon, \theta) , \tag{34}
\]

so that the parameters \(\lambda_\alpha(\epsilon)\) are obtained from the self-consistent equation (at fixed energy \(\epsilon\))

\[
v_\alpha(\eta_p, \theta) = \lambda_\epsilon v_\alpha(\eta_p, \theta) - \frac{\pi \gamma}{\hbar} \lambda_\epsilon \sum_{\eta_p'} \int_{-\theta_0}^{\theta_0} d\theta' \rho(\theta') [1 + \cos(\theta - \theta')] v_\alpha(\eta_p', \theta') \tau_\epsilon(\theta') \tag{35}
\]
where \( v_\alpha(\eta_p, \theta) \) is defined in Eq. (8). From Eq. (14) and (21), we finally get

\[
v_\alpha(\eta_p, \theta) = \lambda_\alpha v_\alpha(\eta_p, \theta) - \frac{\lambda_\alpha}{2 I_1(\delta)} \sum_{\eta_p'=\pm}^\theta \int_{-\theta}^{\theta} d\theta' \frac{1 + \cos(\theta - \theta')} {1 + r(\delta) \cos \theta' \sqrt{\cos \theta' - \delta}} v_\alpha(\eta_p', \theta').
\]

(36)

We now consider the two directions \( \alpha = x, y \) separately.

**Along the x direction**, since the velocity is an odd function of \( \vec{k} \), the sum over \( \eta_p \) in Eq. (36) vanishes: we obtain

\[
\lambda_y(\delta) = \frac{1}{1 - \mathcal{I}_2(\delta)/I_1(\delta)}
\]

(37)

where

\[
\mathcal{I}_2(\delta) = \int_{-\theta_0}^{\theta_0} d\theta \frac{\sin^2 \theta} {\sqrt{\cos \theta - \delta} (1 + r(\delta) \cos \theta)}.
\]

(38)

The function \( I_1(\delta) \) is defined in (13). Note that the expression (37) of the renormalization factor of the transport time \( \lambda_y(\delta) \) reflects the iterative structure of the vertex correction to the bare conductivity that will be obtained within a diagrammatic treatment in section IV B (see Eqs. 66,69). The dependence \( \lambda_y(\delta) \) is plotted in Fig. 6.

![Figure 6](image_url)

**Figure 6.** Dependence on \( \delta = \Delta/\epsilon \) of the renormalization factor of the transport time \( \tau_\alpha^{tr}(\vec{k}) \) with respect to the elastic scattering time: \( \lambda_y(\delta) = \tau_\alpha^{tr}(\vec{k})/\tau_e(\vec{k}) \).

Having obtained the transport times along the \( x \) and \( y \) directions, we now turn to the calculation of the conductivities.

**B. Conductivity**

We can express the current density \( \vec{j} \) occurring in response to the application of the electric field \( \vec{E} \) as

\[
\vec{j} = \int \frac{d^2\vec{k}}{(2\pi)^2} \left[ \left( \vec{k} \right) - n_F(\epsilon_F) \right] (-e\vec{v}(\vec{k}))
\]

(39)

By using \( \partial n_F/\partial \epsilon \simeq -\delta(\epsilon - \epsilon_F) \) and the ansatz (30) for the distribution function \( f(\vec{k}) \) we obtain

\[
\vec{j} = e^2 \sum_{\eta_p=\pm} \int_{-\theta_0}^{\theta_0} d\theta \rho(\epsilon_F, \theta) \vec{v}(\epsilon_F, \eta_p, \theta) \left[ \Lambda(\epsilon_F, \eta_p, \theta), \vec{E} \right].
\]

(40)

The symmetries of this equation imply that off-diagonal terms of the conductivity tensor vanish \( (\sigma_{\alpha,\beta} = 0) \) while the diagonal terms can be written as

\[
\sigma_{\alpha\alpha} = 2e^2 \int_{-\theta_0}^{\theta_0} d\theta \rho(\epsilon_F, \theta) v_\alpha(\epsilon_F, \theta) \Lambda(\epsilon_F, \eta_p, \theta).
\]

(41)

where the factor 2 originates from the two possible signs of \( \eta_p = \pm \). We end up with the Einstein relation

\[
\sigma_{\alpha\alpha} = e^2 \rho(\epsilon_F) D_\alpha,
\]

(42)

with the diffusion coefficients

\[
D_\alpha = 2\lambda_\alpha(\epsilon_F) \int_{-\theta_0}^{\theta_0} d\theta \rho(\epsilon_F, \theta) v_\alpha^2(\theta) \tau_e(\theta)
\]

(43a)

\[
= \langle v_\alpha^2(\epsilon_F, \theta) \tau_e(\epsilon_F, \theta) \rangle_g
\]

(43b)

\[
= \lambda_\alpha(\epsilon_F) \langle v_\alpha^2(\epsilon_F, \theta) \tau_e(\epsilon_F, \theta) \rangle_g.
\]

(43c)

where we have defined the average along the constant energy contour \( \langle \cdots \rangle_g = 2 \int_{-\theta_0}^{\theta_0} d\theta \cdots \rho(\epsilon_F, \theta)/\rho(\epsilon_F) \). This corresponds to the result announced in the introduction: the diffusion coefficients \( D_\alpha \) are obtained by an average over the Fermi surface of \( v_\alpha^2 \tau_e(\theta) \) instead of \( v_\alpha^2 \tau_e \). With our solution of the Boltzmann equation, this difference is accounted for by a renormalization factor \( \lambda(\epsilon_F) \) of the diffusion coefficients, which does not depend on the direction along the Fermi surface but on the direction of application of the electric field. We now specify explicitly the conductivities along the two directions \( x \) and \( y \).

**Along the x direction**, there is no renormalization of the transport time \( (\lambda_x = 1, \tau_x^{tr} = \tau_e) \) and the conductivity
conductivity. We then turn to the calculation of the ring in these other problems. In the next subsections, an understanding of the technicalities naturally occurs in the present paper. Nevertheless our work provides a physical picture of the Boltzmann equation and recover exactly the results of this work. We discuss them in section V. In the B. Diagrammatic approach

IV. DIAGRAMMATIC APPROACH

An alternative approach to describe the diffusive transport of electron consists in a perturbative expansion in disorder of the conductivity tensor using a diagrammatic technique. By confirming the ansatz made to solve the Boltzmann equation and recover exactly the results of Eqs. (44, 46).

A. Green's functions and self-energy

The retarded and advanced Green's functions are defined by:

\[ G^{R/A}(\vec{k}, \vec{k}', \epsilon_F) = \frac{1}{(\epsilon_F - i0)\mathbf{I} - H^0(\vec{k}) \delta(\vec{k} - \vec{k}') - V(\vec{k}, \vec{k}')\mathbf{I}} \]

In the case of the model without disorder defined by Eq. (4), the Green's function is expressed as a 2 × 2 matrix:

\[ G^0(\vec{k}, \epsilon) = \left( \epsilon \mathbf{I} - H^0(\vec{k}) \right)^{-1} \]

where \( \mathbf{I} \) is the identity matrix. Disorder is perturbatively incorporated in the averaged Green’s G function through a self-energy matrix \( \Sigma(\vec{k}, \epsilon) \) such that

\[ \Sigma(\vec{k}, \epsilon) = \int \frac{d\vec{k}}{(2\pi)^2} V(\vec{k}') V(-\vec{k}') G^0(\vec{k} - \vec{k}', \epsilon) \]

Its imaginary part is then obtained as

\[ -\text{Im} \Sigma(\epsilon) = \pi \gamma \int_{-\theta_0}^{\theta} d\sigma \rho(\epsilon, \theta) [\mathbf{I} - \cos \theta \sigma_x] \]

The densities of states \( \rho(\epsilon) \) and \( \rho(\epsilon) \) are given in (13).

For the conductivity along the y direction, the renormalization of the transport time is given by (37) and we obtain

\[ \sigma_y = e^2 \frac{h}{\pi \gamma} \frac{\epsilon^2 \gamma}{I_2(\Delta/e)} \]

where the functions \( I_1(\delta) \) and \( I_2(\delta) \) are respectively given by Eqs. (13) and (38). Eqs. (44, 46) constitute the main results of this work. We discuss them in section V. In the next section, we use a diagrammatic approach which proposes a complementary description of the anisotropy of transport and allows to confirm the ansatz made to solve the Boltzmann equation and recover exactly the results of Eqs. (44, 46).

The real part of the self-energy has been neglected. The elastic scattering rates will be defined below from the imaginary part of the self-energy. To lowest order in the \( \gamma \) this self-energy, solution of a Dyson equation, reads

\[ \Sigma(\vec{k}, \epsilon) = \int \frac{d\vec{k}}{(2\pi)^2} V(\vec{k}') V(-\vec{k}') G^0(\vec{k} - \vec{k}', \epsilon) \]

The real part of the self-energy has been neglected. The elastic scattering rates will be defined below from the imaginary part of the self-energy. To lowest order in the \( \gamma \), this self-energy, solution of a Dyson equation, reads

\[ \Sigma(\vec{k}, \epsilon) = \int \frac{d\vec{k}}{(2\pi)^2} V(\vec{k}') V(-\vec{k}') G^0(\vec{k} - \vec{k}', \epsilon) \]
The discrepancy between diagrammatically on Fig. 8 and lead to mine the averaged classical conductivity are represented where expanding the Green’s function in the disorder potential order amplitude of the conductivity (53) is obtained by ∑ and momentum quantum numbers : Tr = tr

J. F. Figure 7. Conventions for the diagrammatic representation of perturbation theory of transport.

Figure 8. Diagrammatic representation of the classical conductivity with the conventions of Fig. 7. The renormalized current operator is defined in Fig. 9.

**B. Conductivity**

1. **Kubo formula**

The longitudinal conductivity can be deduced from the Kubo formula (α = x, y) :

\[ \sigma_{\alpha\alpha} = \frac{h}{2\pi L^2} \text{Tr} \left[ J_\alpha(\vec{k}) G^R(\vec{k}, \vec{k}, \epsilon_F) J_\alpha(\vec{k}) G^A(\vec{k}, \vec{k}, \epsilon_F) \right], \]

where Tr corresponds to a trace over the pseudo-spin and momentum quantum numbers : Tr = tr \sum \kappa \simeq L^2 \text{tr} \int d\vec{k}/(2\pi)^2 and tr is a trace over the pseudo-spin indices only. For clarity, throughout this section on transport coefficients, we will omit the dependence on the Fermi energy \( \epsilon_F \) of various quantities. The current density operators are also operators acting on both spin and momentum spaces. They are deduced from the Hamiltonian (4) as:

\[ j_x(\vec{k}) = -\frac{e}{m} \hbar k_x \sigma_x, \quad j_y(\vec{k}) = -e c_{\alpha\alpha} \sigma_y. \] (54)

Note that \( j_x \) is linear in momentum while \( j_y \) depends only on spin quantum numbers. Perturbation in the disorder amplitude of the conductivity (53) is obtained by expanding the Green’s function in the disorder potential \( V \) before averaging over the gaussian distribution. In the classical diffusive limit, the dominant terms which determine the averaged classical conductivity are represented diagrammatically on Fig. 8 and lead to

\[ \sigma_{\alpha\alpha} = \frac{h}{2\pi L^2} \text{Tr} \left[ J_\alpha G^R(\vec{k}) J_\alpha G^A(\vec{k}) \right] \] (55)

where \( J_\alpha \) is the renormalized current density operator. The discrepancy between \( J_\alpha \) and the bare current operator \( j_\alpha \) accounts for the appearance of transport time \( \tau^T \) in the Boltzmann approach due to the anisotropy of scattering. This renormalized current operator is easier to define diagrammatically, as shown on Fig. 9.

2. **Conductivity along x**

In this direction, the current operator is linear in \( k_x \), while the averaged Green’s functions \( G^R(\vec{k}), G^A(\vec{k}) \) are even functions of \( k_x \). Hence all the terms in the expression of the renormalized current \( j_x \) with at least a Green’s function vanish by \( k_x \to -k_x \) symmetry, and

\[ j_x(\vec{k}) = j_x(\vec{k}) = -\frac{e}{\hbar} k_x \sigma_x. \] (56)

There is no renormalization of the current operator, in agreement with the result \( \tau^{\alpha\beta} = \tau_\alpha \) from the Boltzmann equation approach. In the \( x \) direction, the expression (55) reduces to

\[ \sigma_{xx} = \left( \frac{he}{m} \right)^2 \frac{\hbar}{2\pi L^2} \text{Tr} \left[ k_x^2 \sigma_x G^R(\vec{k}) \sigma_x G^A(\vec{k}) \right]. \] (57)

Using \( L^{-2} \sum \kappa \simeq \int \rho(\epsilon, \theta) d\epsilon d\theta \) and the parametrization defined in Eq. (6) of the contours of constant energy \( \epsilon \) we perform the integration over energy to obtain

\[ \sigma_{xx} = \frac{e^2}{m} \int_{-\theta_0}^{+\theta_0} d\theta \frac{\rho(\epsilon, \theta) (\cos \theta - \delta)}{1 + \tau(\delta) \cos \theta} \cos \theta \left[ \sigma_x \left[ 1 + \cos \theta \sigma_x + \sin \theta \sigma_y \right] \sigma_x \left[ 1 + \cos \theta \sigma_x + \sin \theta \sigma_y \right] \right]. \]

Performing the spin trace first, we obtain

\[ \sigma_{xx} = \frac{4e^2}{m} \int_{-\theta_0}^{+\theta_0} d\theta \frac{\rho(\epsilon, \theta) (\cos \theta - \delta)}{1 + \tau(\delta) \cos \theta} \cos^2 \theta. \] (58)

By using eq. (14) for the directional density of states we recover exactly the integral expression for the result (44) of Boltzmann approach:

\[ \sigma_{xx} = \frac{e^2}{m} \int_{-\theta_0}^{+\theta_0} d\theta \frac{\rho(\epsilon, \theta) (\cos \theta - \delta)}{1 + \tau(\delta) \cos \theta} \cos^2 \theta. \] (59)

3. **Renormalized current operator along y**

In the \( y \) direction, the current operator is renormalized : the bare current operator \( j_y \) is independent of the momentum \( \vec{k} \) and the symmetry argument used for the \( x \) direction does not hold anymore. This renormalized current operator satisfies a Bethe-Salpeter equation represented in Fig. 9:

\[ J_y = j_y + J_y \Pi \gamma \] (60)
where tensor product in spin space are assumed and
\[ \Pi(\epsilon, \Delta) = \int \frac{d\epsilon'}{(2\pi)^2} G^R(\epsilon', \epsilon) \otimes G^A(\epsilon', \epsilon) \cdots. \] (61)

Due to the spinorial structure of the wave functions, this propagator is here an operator acting as the tensor product of two spin \( \frac{1}{2} \) spaces. The notation \( \cdots^T \) corresponds to a transposition of spin matrices. Using the parametrization defined in Eq. (6) of the contours of constant energy \( \epsilon \) we perform the integration over energy to obtain for \( \Pi(\epsilon, \Delta) \equiv \Pi(\delta = \Delta/\epsilon) \):
\[ \Pi(\delta) = \frac{\pi \tau_0}{h} \int_{-\theta_0}^{+\theta_0} d\theta \frac{\rho(\epsilon, \theta)}{1 + r(\delta) \cos \theta} \times [I + \cos \theta \sigma_x + \sin \theta \sigma_y] \otimes [I + \cos \theta \sigma_x - \sin \theta \sigma_y]. \] (62)

The expression (14) for the directional density of states allows to rewrite it as
\[ \Pi(\delta) = \frac{1}{2\gamma I_1(\delta)} \left[ I_2(\delta) I \otimes I + (I_1(\delta) - I_2(\delta)) \sigma_x \otimes \sigma_x - \mathcal{J}_2(\delta) \sigma_y \otimes \sigma_y + \mathcal{J}_1(\delta) (I \otimes \sigma_x + \sigma_x \otimes I) \right], \] (63)
where we introduced the functions:
\[ I_1(\delta) = \int_{-\theta_0}^{\theta_0} d\theta \frac{1}{\sqrt{\cos \theta - \delta (1 + r(\delta) \cos \theta)}}, \] (64)
\[ I_2(\delta) = \int_{-\theta_0}^{\theta_0} d\theta \frac{\cos \theta}{\sqrt{\cos \theta - \delta (1 + r(\delta) \cos \theta)}}, \] (65)
whereas \( I_1 \) and \( I_2 \) are defined in Eqs. (13,38).

The inversion of the Bethe-Salpeter equation (60) is done in the appendix A and we find
\[ J_y = J_y (I \otimes I - \gamma \Pi(\delta))^{-1} = \left(1 - \frac{I_2(\delta)}{I_1(\delta)} \right)^{-1} J_y. \] (66)

4. Conductivity along \( y \)

Following the formula (55), the average conductivity along \( y \) is expressed as
\[ \overline{\sigma}_{yy} = \frac{\hbar}{2\pi} \text{tr} [J_y, \Pi(\delta), J_y]. \] (67)

From the eq. (60), we express \( J_y, \Pi(\delta) = \gamma^{-1} (J_y - j_y) \) to obtain from (67):
\[ \overline{\sigma}_{yy} = \frac{\hbar}{2\pi \gamma} \text{tr} [(J_y - j_y) j_y]. \] (68)

The expression for the renormalized current operator (66) leads to the final result
\[ \overline{\sigma}_{yy} = \frac{e^2 \hbar \gamma^2}{\pi \gamma} \frac{I_2(\delta)}{I_1(\delta) - I_2(\delta)}, \] (69)
which is precisely the result (46) obtained within the Boltzmann equation approach.

This concludes the derivation of the conductivity tensor within the diagrammatic approach. In doing so, we have identified the encoding of the anisotropic scattering rates through the matrix self-energy (52), while the corresponding transport times are hidden into the renormalization of vertex operators (56,66). Comparison with the Boltzmann approach allows to unveil the physical meaning of these technical structures, which we believe to be applicable to other situations of anisotropic transport of Dirac-like states.

V. RESULTS AND DISCUSSION

We now turn to a discussion of our results for various situations corresponding to energy spectra represented in Fig. 2.
A. $\Delta = 0$ : Semi-Dirac spectrum

Focusing first on the merging point ($\Delta = 0$), we find that the conductivities are expressed, from Eqs. (44, 46, 59, 69) as:

$$
\sigma_{xx}(\epsilon) = \frac{e^2}{2} \frac{\Delta}{\gamma m} \frac{I_3(0)}{I_1(0)} \approx 0.197 \frac{e^2}{\gamma m} \frac{\Delta}{\gamma m} \quad (70a)
$$

$$
\sigma_{yy}(\epsilon) = \frac{e^2}{2 \gamma c_y^2} \frac{I_2(0)}{I_1(0) - I_2(0)} \approx 1.491 \frac{e^2}{\gamma c_y^2} \frac{\Delta}{\gamma m} \quad (70b)
$$

This case, which corresponds to an hybrid dispersion relation, linear in one direction and quadratic in the other direction, has been previously studied in Ref. 34. However these authors have neglected both the spindorial structure of the wave function and the angular dependence of the elastic scattering time caused by the anisotropic dispersion, whose importance is emphasized in the present paper. Using the numerical values of the integrals given in appendix B, we find $\lambda_y(0) \approx 2.4915$ and $\lambda_y(0) \approx 2.4915$:

$$
\sigma_{xx} = \frac{I_3(0)}{I_3(0)} \frac{\Delta}{\gamma m} \approx 0.781 \frac{\Delta}{\gamma m} \quad (71a)
$$

$$
\sigma_{yy} = \lambda_y(0) \frac{I_2(0)}{I_2(0)} \frac{\Delta}{\gamma m} \approx 2.237 \frac{\Delta}{\gamma m} \quad (71b)
$$

where $\sigma_{xx}^B$ and $\sigma_{yy}^B$ are the values obtained in Ref. [34].

The energy dependence of the conductivities (70) arises from the energy dependence of the average squared velocities. It is therefore independent of the energy along the $y$ direction, while it increases linearly with energy along the $x$ direction.

B. $\Delta > 0$ : gapped spectrum

When $\Delta > 0$, the energy spectrum exhibits a gap and we study here the conductivity above this gap at energies $\epsilon > \Delta$. Along the $x$ direction, the renormalization factor $\lambda_x = 1$ so that $\tau^x_x(\theta) = \tau_0(\theta)$. The energy dependence arises mainly from the energy dependence of the average squared velocity. Therefore we expect a roughly linear dependence in energy $\Delta$:

$$
\sigma_{xx}(\epsilon) = \frac{e^2}{2} \frac{\Delta}{\gamma m} \frac{I_3(\Delta/\epsilon)}{I_1(\Delta/\epsilon)} \approx 0.2 \frac{e^2}{\gamma m} \frac{\Delta}{\epsilon - \Delta} \quad (72)
$$

$$
\approx 2 \frac{e^2}{\gamma m} \frac{\Delta}{\epsilon - \Delta} \quad (73)
$$

where $c_x = \sqrt{2|\Delta/m}$ is the velocity along $x$ of the massive Dirac equation describing the spectrum for small momenta.

The dependence in energy of the conductivity $\sigma_{yy}$ is mainly due to the energy dependence of the renormalization factor $\lambda_y$ between transport time and relaxation time:

$$
\sigma_{yy}(\epsilon) = \frac{e^2}{2} \frac{\Delta}{\gamma m} \frac{I_2(\Delta/\epsilon)}{I_1(\Delta/\epsilon)} \approx \frac{e^2}{\gamma m} \frac{\Delta}{\epsilon - \Delta} \quad (74)
$$

$$
\approx \frac{e^2}{\gamma m} \frac{\Delta}{\epsilon - \Delta} \quad (75)
$$

The energy dependence of the conductivities $\sigma_{xx}$ and $\sigma_{yy}$ is plotted in Fig. 10.

![Figure 10](image)

C. $\Delta < 0$ : Dirac spectrum

When $\Delta < 0$, the conductivity vanishes at the saddle point ($\Delta = 0$), the conductivity vanishes at the saddle point ($\Delta = 0$) as functions of $\epsilon/\Delta$ in the gapped phase ($\Delta > 0$). The energy dependence of $\sigma_{xy}$ arises from the energy dependence of the velocity along $x$, while for $\sigma_{yy}$ it comes mainly from the energy dependence of the renormalization factor $\lambda_y$.

![Figure 11](image)

In this phase, we have two regimes separated by the saddle point energy $|\Delta|$. At high energy above the sad-
dle point, $\epsilon \gg |\Delta|$, the energy dependence of the conductivities are still given by Eqs. (73, 75). In the low energy limit $\epsilon \ll |\Delta|$, expanding these expressions using Eq. (B17), we recover the conductivities associated to a conic dispersion of characteristic velocities $c_x$ and $c_y$:

$$\sigma_{xx}(\epsilon \to 0) = \frac{e^2 h}{\pi \gamma} c_x^2$$

(76)

$$\sigma_{yy}(\epsilon \to 0) = 2 \frac{e^2 h}{\pi \gamma} c_y^2.$$

(77)

Note however the factor 2 between the two expressions. This is due to the fact that $\tau_{tr}^x = 2\tau_e$ like in graphene while $\tau_{tr}^y = \tau_e$. It is instructive to compare with this limit with the case of graphene, where it is known that $\tau_{tr} = 2\tau_e$ is all directions$^{33}$, and where Einstein relation $\sigma_{\alpha\alpha} = e^2 (c_\alpha^2 \tau_{tr}/2) \rho(\epsilon_F)$ together with the Fermi golden rule $\tau_{tr} = 2\tau_e = 2\hbar/(\pi \rho(\epsilon_F)\gamma)$ leads to

$$\sigma(\text{graphene}) = \frac{e^2 h}{\pi \gamma} v_F^2.$$

(78)

Using the fact that $c_x^2 = c_y^2 = v_F^2/2$, we find the same result for $\sigma_{yy}$ but the conductivity is twice smaller along the $x$ direction. The difference by a factor 2 between $\sigma_{xx}$ and $\sigma_{yy}$ results from intervalley scattering taking place along the $x$ direction (see Ref. 33 or a related discussion of diffusion within graphene with different intervalley and intravalley disorder rates).

It is important to note that our calculations predict vanishing conductivities at the saddle point $\epsilon = |\Delta|$. That is the result of the logarithmic divergence of the density of states producing a vanishing elastic scattering time in Eq. (21). However, in such a limit, $k_F l_e \to 0$, so our approximations are no longer valid. To describe correctly the behavior of the scattering time in the vicinity of the saddle point, it is necessary to go beyond second order perturbation theory, using for instance the self-consistent Born approximation$^{37}$, in order to obtain a finite density of states and a non-zero elastic scattering time. Qualitatively, we expect that the zero of the conductivity will be replaced by a minimum for $\epsilon \simeq |\Delta|$.

D. Evolution of conductivities across the transition

We are now in position to discuss the evolution of the conductivity at fixed energy $\epsilon_F$, as a function of the parameter $\Delta$ as we cross the merging transition. Such evolution, derived for eq. (44,46) is represented on Fig. 12, where we have plotted $\sigma_{\alpha\alpha}$ in units of $e^2 h c_\alpha^2/\gamma$ for $\alpha = x, y$ and $\tilde{c}_x = \sqrt{2\epsilon_F/m}$ and $\tilde{c}_y = c_y$. Below the saddle point for $\Delta < -\epsilon_F$, $\sigma_{yy}$ is nearly constant, while $\sigma_{xx}$ decreases almost linearly with $\Delta$. At the saddle point $\Delta = -\epsilon_F$ where the topology of the Fermi surface changes, a dip in both $\sigma_{xx}$ and $\sigma_{yy}$ is visible, down to minimal values not quantitatively captured by the present approach. Past the saddle point, while $\sigma_{xx}$ remains linearly decreasing with $\Delta$, albeit more slowly, $\sigma_{yy}$ is first increasing, presenting a maximum for $\Delta/\epsilon_F \simeq -0.39$ and then decreases to zero. No signature of the underlying transition at $\Delta = 0$ is manifest in the transport at high Fermi energy $\epsilon_F$.

![Figure 12. Conductivities (in units of $e^2 h c_\alpha^2/\gamma$ for $\alpha = x, y$) as a function of the parameter $\Delta$ for a fixed chemical potential $\epsilon$. The conductivity $\sigma_{xx}$ decreases monotonically with $\Delta$, in almost linear fashion with a change of slope at the saddle point $S$. The conductivity $\sigma_{yy}$ is almost constant below the saddle point. Above the saddle point, the behavior of $\sigma_{yy}$ becomes non-monotonous with $\Delta$. At the metal-insulator transition, both $\sigma_{xx}$ and $\sigma_{yy}$ vanish linearly. Symbols (a), (b), (c), M and S refer to the regions presented in Fig. 2.](image)

VI. CONCLUSION

We have studied the behavior of the conductivity in both the Dirac phase, the critical semi-Dirac and above the gapped phase. Using the complementary Boltzmann and diagrammatic techniques we have identified the different nature of anisotropy of the elastic scattering times and transport times. Indeed the transport is inherently anisotropic due both to the spinorial structure of the eigenstates and the anisotropy of the dispersion relation. The approaches developed in this paper can be generalized to study the diffusive transport in other semimetallic phases, including the various three dimensional species recently identified.

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Then the equation (A5) provides the expression for the renormalized current operator:

\[ J_y = j_y \left( I \otimes I - \gamma \Pi(\delta) \right)^{-1} = \left( 1 - \frac{I_2(\delta)}{I_1(\delta)} \right)^{-1} J_y . \] (A7)

A word of caution is necessary at this stage: \((1 - \gamma \Pi(\delta))^{-1}\) is the structure factor which encodes the propagation of the diffuson modes\(^{31}\). In the symplectic class which we consider, there is one such mode which is diffusive: \(1 - \gamma \Pi(\delta)\) possesses a vanishing eigenvalue \(\propto (Dq^2)\). Hence in the limit \(q \to 0\) that we consider, \(1 - \gamma \Pi\) is no longer invertible. In principle, we should have kept a finite momentum \(q\) during the calculation, and taken the limit \(q \to 0\) only in the result. However, the vertex renormalization that we consider in this section is not sensitive to this long-wavelength physics: it corresponds to a renormalization of the elastic scattering time into a transport time, which occurs on short distances. This is manifest in the independence of the result (A5) on the determinant \(\Delta\) of the matrix \(M\): this is a classical contribution, which depends on these massive diffusion modes, while the diffusive long distance modes enter the quantum correction not discussed in this paper.

### Appendix B: Special Functions

In this appendix, we discuss a few useful results of the various integrals entering the expressions of transport coefficients in the paper and arising as integrals along the constant energy contours of the model. Let us first consider the integrals:

\[ I_1(\delta) = \int_{-\theta_0}^{\theta_0} \frac{d\theta}{\cos \theta - \delta} , \quad J_1(\delta) = \int_{-\theta_0}^{\theta_0} \frac{d\theta \cos \theta}{\sqrt{1 - \delta}} , \]

with \(\cos \theta_0 = \delta\) if \(|\delta| < 1\) and \(\theta_0 = \pi\) otherwise. Defining \(X = \sqrt{2/(1 - \delta)}\), we find\(^{38}\):

\[ I_1(\delta) = \frac{4}{\sqrt{1 - \delta}} K(X) \quad \delta < -1 \] (B1)

\[ I_1(\delta) = 2\sqrt{2} K(1/X) \quad -1 < \delta < 1 \] (B2)

and

\[ J_1(\delta) = \frac{4}{\sqrt{1 - \delta}} \left[ (1 - \delta) E(X) + \delta K(X) \right] \text{ for } \delta < -1 , \] (B3)

and

\[ J_1(\delta) = 2\sqrt{2} \left[ 2E(1/X) - K(1/X) \right] \text{ for } -1 < \delta < 1 . \] (B4)

The anisotropy factor \(r(\delta) = J_1(\delta)/I_1(\delta)\) reads:

\[ r(\delta) = (1 - \delta) E(X)/K(X) + \delta \quad \text{for } \delta < -1 \] (B5)

\[ r(\delta) = 2E(1/X)/K(1/X) - 1 \quad \text{for } -1 < \delta < 1 . \] (B6)
The functions $I_1(\delta)$ and $J_1(\delta)$ are plotted in Fig. 13, and the dependence on $\delta$ of $r(\delta)$ is shown on Fig. 5.

Figure 13. Functions $I_1(\delta)$ and $J_1(\delta)$

Figure 14. Functions $I_1(\delta)$, $J_1(\delta)$, $I_2(\delta)$ and $I_3(\delta)$

Let us now consider the four integrals

\[ I_1(r, \delta) = \int_{\theta_0}^{\theta} \frac{d\theta}{1 + r \cos \theta \sqrt{\cos \theta - \delta}} \]  
\[ J_1(r, \delta) = \int_{\theta_0}^{\theta} d\theta \cos \theta \]  
\[ I_2(r, \delta) = \int_{\theta_0}^{\theta} \frac{d\theta \sin^2 \theta}{1 + r \cos \theta \sqrt{\cos \theta - \delta}} \]  
\[ I_3(r, \delta) = \int_{\theta_0}^{\theta} \frac{d\theta \cos^2 \theta \sqrt{\cos \theta - \delta}}{1 + r \cos \theta} \]

We first focus on first the integral $I_1(r, \delta)$. For $\delta < -1$, it can be rewritten as:

\[ I_1(r, \delta) = \frac{4}{(1 + r) \sqrt{1 - \delta}} \]

\[ \int_0^{\frac{\pi}{2}} \frac{d\theta}{1 - \frac{2r}{1+r} \sin^2 \theta \sqrt{1 - \frac{2}{1+\delta} \sin^2 \theta}} \]

\[ = \frac{4}{(1 + r) \sqrt{1 - \delta}} \Pi \left( \frac{\pi}{2} \frac{2r}{1+r} \sqrt{\frac{2}{1 - \delta}} \right) \]

where $\Pi$ is an elliptic integral of the third kind. For $|\delta| < 1$, we use the change of variable $\sin \frac{\theta}{2} = \sin \frac{\theta_0}{2} \sin \varphi$ to rewrite this function as:

\[ I_1(r, \delta) = \frac{2\sqrt{2}}{1 + r} \int_0^{\frac{\pi}{2}} \frac{d\varphi}{1 - \frac{2r}{1+r} \sin^2 \frac{\theta_0}{2} \sin^2 \varphi \sqrt{1 - \sin^2 \frac{\theta_0}{2} \sin^2 \varphi}} \]

\[ = \frac{2\sqrt{2}}{1 + r} \Pi \left( \frac{\pi}{2} \frac{2r}{1+r} \sin \frac{\theta_0}{2} \right) . \]  

(B13)

Moreover the integrals $J_1(r, \delta), I_2(r, \delta)$ and $I_3(r, \delta)$ can be expressed in terms of $I_1(\delta), J_1(\delta)$ and $I_1(r, \delta)$:

\[ J_1(r, \delta) = \frac{1}{r} \left[ I_1(\delta) - I_1(r, \delta) \right] , \]  

(B14)

\[ I_2(r, \delta) = \frac{1}{r^2} I_1(\delta) - \frac{1}{r} J_1(\delta) + \left( 1 - \frac{1}{r^2} \right) I_1(r, \delta) , \]  

(B15)

\[ I_3(r, \delta) = \frac{1}{r} \left( \frac{1}{3} + \frac{\delta}{r} + \frac{1}{r^2} \right) I_1(\delta) - \frac{1}{r} \left( \frac{\delta}{3} + \frac{1}{r} \right) J_1(\delta) \]

\[ - \frac{1}{r^2} \left( \delta + \frac{1}{r} \right) I_1(r, \delta) . \]  

(B16)

Finally, the integrals used in the text are

\[ I_1(\delta) = I_1[r(\delta), \delta] \]

\[ J_1(\delta) = J_1[r(\delta), \delta] \]

\[ I_2(\delta) = I_2[r(\delta), \delta] \]

\[ I_3(\delta) = I_3[r(\delta), \delta] . \]

(B17)

The following special values are of particular interest for the expressions in the text :

\[ I_1(0) = 2\sqrt{2}K \left( \frac{1}{\sqrt{2}} \right) \approx 5.2441 \]

\[ J_1(0) = \pi \sqrt{2}/K \left( \frac{1}{\sqrt{2}} \right) \approx 2.3963 \]

\[ r(0) = J_1(0)/I_1(0) \approx 0.457 \]

\[ I_2(0) = \frac{4}{3} \sqrt{2}K(1/\sqrt{2}) \approx 3.4961 \]

\[ I_3(0) \approx 3.1393 \]

\[ I_3(0) \approx 1.4377 \]

\[ I_3(0) \approx 1.0322 . \]

as well as the limits when $\delta \to -\infty$ :

\[ \frac{I_2(\delta)}{I_1(\delta) - I_2(\delta)} \to 1; \quad \frac{I_3(\delta)}{I_1(\delta)} \to \frac{\delta}{2} . \]

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35. Note the correspondance between our notations $I_k(x)$, $(k = 1, 2, 3)$ and those $I_k$ of Ref. 34 : $I_k(0) = 4I_k$.

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