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# Quantum corrections in the Boltzmann conductivity of graphene and their sensitivity to the choice of formalism

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**Abstract.** Semiclassical spin-coherent kinetic equations can be derived from quantum theory by many different approaches (Liouville equation based approaches, nonequilibrium Green's function techniques, etc). The collision integrals turn out to be formally different, but coincide in textbook examples as well as for systems where the spin-orbit coupling is only a small part of the kinetic energy like in related studies on the spin Hall effect. In Dirac cone physics (graphene, surface states of topological insulators like  $\text{Bi}_{1-x}\text{Sb}_x$ ,  $\text{Bi}_2\text{Te}_3$  etc), where this coupling constitutes the entire kinetic energy, the difference manifests itself in the precise value of the electron-hole coherence originated quantum correction to the Drude conductivity  $\sigma_0 \sim (e^2/h)\ell k_F$ . The leading correction is derived analytically for single and multilayer graphene with general scalar impurities. The often neglected principal value terms in the collision integral are important. Neglecting them yields a leading correction of order  $(\ell k_F)^{-1}$ , whereas including them can give a correction of order  $(\ell k_F)^0$ . The latter opens up a counterintuitive scenario with finite electron-hole coherent effects at Fermi energies arbitrarily far above the neutrality point regime, for example in the form of a shift  $\delta\sigma \sim e^2/h$  that only depends on the dielectric constant. This residual conductivity, possibly related to the one observed in recent experiments, depends crucially on the approach and could offer a setting for experimentally singling out one of the candidates. Concerning the different formalisms we notice that the discrepancy between a density matrix approach and a Green's function approach is removed if the generalized Kadanoff-Baym Ansatz in the latter is

replaced by an anti-ordered version. This issue of Ansatz may also be important for Boltzmann type treatments of graphene beyond a linear response.

**Keywords:** exact results, graphene (theory), Boltzmann equation, quantum transport

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## 1. Introduction

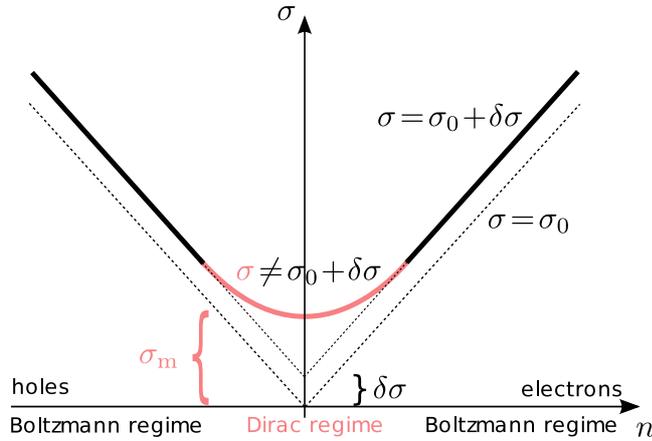
Since the first isolation of graphene in 2004 [1] the electrical conductivity of this system has attracted huge attention. To a good approximation the electrons can be described as massless 2d Dirac electrons for which the spin-orbit interaction that yields the characteristic Dirac cone is given by the pseudospin derived from the bipartite honeycomb lattice [2, 3]. The conical electron and hole bands touch at the Dirac points. The Brillouin zone contains two inequivalent degenerate Dirac points—K and K'—that give an additional valley index. Finally there is the ordinary electron spin. To a first approximation, the conductive properties of graphene involve only the pseudospin in a non-trivial way.

The main focus has been on undoped graphene, with the chemical potential exactly at the degenerate Dirac points. This regime of chemical potential close to zero—the Dirac regime—hosts the most exotic features, for example the finite conductivity minimum at seemingly zero charge carrier density [4, 5]. Quantum effects due to electron-hole coherence (that is, pseudospin coherence) like Zitterbewegung can dictate the observed conductivity even to lowest approximation [6]. We refer to [7] for a review on early work on the Dirac regime.

Away from the Dirac regime, with a large enough charge carrier density there is a crossover into the Boltzmann regime  $\ell k_F \gg 1$  (with  $\ell$  the mean free path and  $\hbar k_F$  the Fermi momentum). Here, the conductivity can be understood to lowest order without taking into account quantum effects, such as electron-hole coherence, and are therefore more intuitive. The crossover between the two regimes has recently been studied numerically [8]–[10].

In many experiments on graphene samples on substrates [4, 5], [11]–[13] the dc conductivity in the Boltzmann regime is observed to be linear in the electron (hole) density (see figure 1). This results in the characteristic V-shape in the conductivity as a function of gate voltage. The linearity is less pronounced in suspended graphene, where the concentration of charged impurities in particular has been reduced [14, 15]. Theoretically the linear behavior is well described by the ordinary Drude conductivity  $4\sigma_0 = 4(e^2/2h)\ell k_F$  derived from a Boltzmann equation with four degenerate (valley and real spin) incoherent bands, provided that screened charged impurities are assumed [16]–[18]. Point-like impurities on the contrary lead to a Drude conductivity that is independent of charge carrier density and therefore this model fails even on a qualitative level [19]. As one expects the charge carrier to be mainly of one type (either electrons or holes), the pseudospin band index can be left aside. With interband coherences neglected, the collision integral contains only transition rates between energy eigenstates. Such rates are simply derived with Fermi's Golden rule. The specific properties of massless Dirac electrons enter into the transition rates merely as a spin-overlap factor due to the chirality of the eigenstates and as a Fermi momentum dependent (and therefore electron density dependent) Thomas-Fermi momentum  $p_{TF}$  due to the linearity of the spectrum. (In a 2DEG with quadratic dispersion the screening length  $\hbar/p_{TF}$  is, in contrast, independent of the Fermi momentum.)

In the Boltzmann regime  $\ell k_F \gg 1$  the electron-hole coherent features of Dirac electrons only manifest themselves if one goes beyond the lowest order result,  $\sigma_0 \propto \ell k_F$ , to look for quantum corrections. A Boltzmann approach to these quantum corrections requires a kinetic equation that is quantum coherent in band indices, for graphene



**Figure 1.** Sketch of the dc conductivity  $\sigma$  in monolayer graphene as a function of the electron density  $n$ , as observed in some experiments [4, 5], [11]–[13], in particular including a residual conductivity  $\delta\sigma$  as observed by Chen *et al* [13]. At the neutrality point  $n = 0$ , the charge density is zero, and one would expect zero charge carrier density at low temperatures. One of the surprises of graphene is the conductivity minimum  $\sigma_m \sim e^2/h$ . In the Dirac regime  $n \approx 0$  (red/gray) the usual criterion  $\ell k_F \gg 1$  for a Boltzmann treatment is not satisfied (at least not for screened charged impurities). Away from the Dirac regime a semiclassical approach should usually apply. The observed linear dependence in the Boltzmann regime (black) is described by the Drude conductivity  $\sigma_0 = 2e^2 \ell k_F / h \propto |n|$  for screened charged impurities. (Point-like impurities, in contrast, yield  $\sigma_0 \propto |n|^0$ . The resistivity due to them starts to compete with that of screened charged impurities for  $|n|$  large enough.) Effects of electron–hole coherence do not enter into the Drude conductivity, and reveal themselves only in quantum corrections of higher order in  $(\ell k_F)^{-1}$ . A contribution  $(\ell k_F)^{-1}$  can explain the initial convexity as one approaches the Dirac regime. A contribution  $(\ell k_F)^0$  enters as a constant shift in the Boltzmann conductivity and contributes thus to the residual conductivity  $\delta\sigma$ . The latter is directly read off by linear extrapolation. A precise knowledge of other contributions to  $\delta\sigma$  (e.g. weak localization, ...), allowing a precise estimate of the electron–hole coherent contribution, would in turn single out one of the many possible derivations discussed in the present paper. With one exception [10] the contribution to the conductivity minimum depends also, in general, on the approach. However, these differences can probably not be studied as cleanly as those in the residual conductivity. We want to stress that the residual conductivity is inherent in the Boltzmann regime whereas the minimum conductivity is inherent in the Dirac regime.

the pseudospin index [20]–[22]. Interband coherent collision integrals are beyond the application range of Fermi’s Golden rule. To access the ‘transition rates’ involving the interband components (a.k.a. off-diagonal, (pseudo)spin-precessing or Zitterbewegung components) in the collision integral, one typically has to resort to a fully quantum coherent theory and then derive a Boltzmann equation by a semiclassical expansion in the space and time variables, but not in the spin, which is to be kept quantum coherent. Common approaches for deriving quantum coherent kinetic equations are density matrix approaches and nonequilibrium Green’s function approaches, both with

further subdivisions. The former start with a single-time density-matrix-type state variable  $\rho(x_1, x_2, t_1)$  governed by a quantum Liouville equation (von Neumann equation). The latter start with a double-time correlator  $G^<(x_1, t_1, x_2, t_2)$  governed by dynamic equations derived from, for example, the Kadanoff–Baym equation or the Keldysh equation. At a later stage some approximation has to be invoked to recover single-time equations. This choice of approximation is the problem of the Ansatz which will be discussed later. All the mentioned treatments of pseudospin coherence induced quantum corrections in graphene use the density matrix approach. In other contexts involving spin-coherent Boltzmann approaches to transport in the presence of spin–orbit coupling, such as the spin Hall effect, Green’s function derivations have also been used [23]–[27]. However, in these cases transport was addressed to leading order rather than quantum corrections. One of the two central questions of this paper is whether the two approaches are equivalent in general, and in particular when addressing quantum corrections to the graphene conductivity.

The general small expansion parameter for quantum corrections in a Boltzmann regime is  $(\ell k_F)^{-1}$ . One example is the famous result by Gorkov *et al* [28] for the correction  $\delta\sigma/\sigma_0 = (\pi\ell k_F)^{-1} \log \omega_0\tau$  due to weak localization. The quantum correction to the graphene Drude conductivity due to electron–hole coherence is no exception<sup>3</sup>. The second central question addressed in this work is whether the series of quantum corrections in powers of  $(\ell k_F)^{-1}$  starts at the order  $(\ell k_F)^{-2}\sigma_0$  or already the order  $(\ell k_F)^{-1}\sigma_0$ . A correction  $\delta\sigma \sim (e^2/h)(\ell k_F)^{-1}$  to the Drude conductivity  $\sigma_0 \sim (e^2/h)\ell k_F$  would depend on impurity concentration and impurity strength. For screened charged impurities in graphene it would increase with decreasing electron density  $n$ , which would explain the onset of convex behavior of the conductivity as one approaches the Dirac regime. Far away from the Dirac regime the contribution becomes arbitrarily small. A contribution of the lower order  $\delta\sigma \sim e^2/h(\ell k_F)^0$  would be independent of the impurity density and impurity strength. At least in monolayer graphene it would also be independent of the electron density, which would appear as a constant shift of the Drude conductivity, as illustrated in figure 1. Electron–hole coherence effects would then remain finite arbitrarily far away from the Dirac regime, which appears rather counterintuitive. References [20, 21] found the leading correction to the dc conductivity to be of the order  $(\ell k_F)^{-1}$  within a pseudospin-coherent Boltzmann approach<sup>4</sup>. Trushin and Schliemann [21] found a leading correction of the same order<sup>5</sup> although their approach was qualitatively different in that they, in contrast to Auslender *et al*, discarded the principal value terms in the pseudospin-coherent collision

<sup>3</sup> We find that this point has not been clearly stated in the previous related studies [20]–[22]. Reference [20] does not seem to discuss such a parameter. Reference [21] introduces the parameter  $\alpha = 4(\ell k_F)^2$  as a ‘novel electron–hole coherence parameter’. Culcer and Winkler’s treatment [22] expanding in the transition rate  $|U_{kk'}|^2$ , clearly displays the origin of the expansion parameter in the spin-coherent context. Only in the preceding paper [26] was it stated that this expansion is one in  $\hbar/\Omega_F\tau$ , where  $\Omega$  is the spin–orbit coupling, however there in a context where  $\Omega_F\tau \ll \epsilon_0\tau \sim \ell k_F$ .

<sup>4</sup> This is Auslender and Katsnelson’s result for small enough impurity concentrations and interaction strengths, the limit of small  $\Phi(\propto 1/\ell k_F)$  in equations (84) and (85) in [20].

<sup>5</sup> This is the correction discussed before equation (19) derived from equations (13) and (14). Notice that Trushin *et al* also discuss another expansion, namely the expansion in the interaction range  $R$ , which is not an expansion in  $1/\ell k_F$ . That they get it to be an expansion in the density is because  $R$  is taken as a constant fitting parameter. In contrast, in the RPA result  $R$  is the inverse of the Thomas–Fermi momentum, which for graphene is proportional to  $k_F$  (see the end of our section 2). In this case the parameter  $Rk_F$  in graphene is independent of  $k_F$  and one cannot expand in the electron density.

integral. (See also [29].) Both papers found the result to be ultraviolet divergent for point-like impurities<sup>6</sup>. Culcer and Winkler [22] studied screened charged impurities. They too neglected principal value terms. They solved their spin-coherent Boltzmann equation only up to order  $(\ell k_F)^0$ , hence the previously found corrections  $\sim(\ell k_F)^{-1}$  were out of reach. However, solving the Boltzmann equation by introducing a frequency dependence lead to a quantum correction  $\delta\sigma(\omega) \sim e^2/h$  for nonzero temperatures. As this correction of order  $(\ell k_F)^0$  vanishes in the zero-frequency limit their result is not inconsistent with that of Trushin *et al* or, at first sight, that of Auslender *et al*.

An important contribution of the paper of Auslender *et al* [20] was that they realized the importance of *principal value terms* and included them in their collision integral for graphene. However, they did not discuss the physical origin or necessity of these terms that so severely complicated their analysis. The subsequent papers [21, 26] neglected them without much comment and this seems to be the rule also in other contexts where Boltzmann approaches are applied to spin-orbit coupled systems, as for example in the spin Hall effect [23]–[27]. In other fields the meaning of these terms in a Boltzmann treatment is rather clear (for the context of strongly interacting fermions see e.g. Lipavsky *et al* [30]). As this does not appear to be the case in the spin-orbit context, we will in the technical sections discuss the physical origin of these terms and thus explain why we insist on keeping them although they make the interpretation of the Boltzmann equation more elusive and also considerable increase the technical challenge of solving these integro-differential equations. An example of this increased complexity is the mathematical *tour de force* of Auslender *et al* [20], and that treatment still applies only to the simplifying case of point-like impurities.

In trying to answer the two aforementioned central questions the present paper has two aims. One aim is to (re)derive a pseudospin-coherent Boltzmann equation and to give a systematic derivation of the leading quantum correction by including the principal value parts, but nonetheless consider the screened charged impurities which are relevant to graphene. We can consider a simpler problem than that of Auslender *et al* by using an iterative scheme in the spirit of Culcer *et al* rather than attempting to solve the equations to all orders in  $(\ell k_F)^{-1}$  in one go. To illustrate the importance of the principal value terms we also solve the same Boltzmann equations with principal value terms neglected. This problem, in contrast, is also easily solved non-recursively [27]. Since we formulate the Boltzmann equation for a spin-orbit coupling of arbitrary winding number  $N$ , the results also apply to certain models [31]–[34] for bilayer and multilayer graphene. Quantum corrections in the bilayer case  $N = 2$  have been considered by Culcer *et al* [35] with a similar approach as in [22]. We will refer to  $N = \pm 1$  as the ‘monolayer case’ and to  $|N| \neq 1$  as the ‘multilayer case’. (Actual  $N$ -layer graphene Hamiltonians can, however, depending on the stacking, be written as tensor products of lower- $N$  Hamiltonians, in some cases including the monolayer  $N = \pm 1$  Hamiltonian [33, 34].) We find the following results:

- (1) With principal value terms neglected, the first quantum correction is of order  $(\ell k_F)^{-1}$  both in the dc conductivity as well as in the dissipative ac conductivity. Higher order

<sup>6</sup> Auslender *et al* treated point-like impurities. Trushin *et al* treated finite range impurities, but expanded in the range parameter  $R$ . The first term in this expansion corresponds to the point-like limit. This issue is readdressed in the appendix of the sequel [29].

corrections beyond the order  $(\ell k_F)^{-1}$  are absent in the monolayer case  $|N| = 1$ , but present to infinite order in the multilayer case  $|N| \neq 1$ .

- (2) With principal value terms included, the leading quantum correction to the dc conductivity is of order  $(\ell k_F)^0$ . In particular it is independent of the impurity concentration and of the impurity strength. For screened charged impurities at a negligible distance from the graphene plane, the correction depends only on the dimensionless parameter  $k_F/k_{TF}$  (with  $\hbar k_F$  the Fermi momentum and  $1/k_{TF}$  the Thomas–Fermi screening length). In the monolayer case  $N = \pm 1$  (with  $k_{TF} \propto k_F$ ) the correction is also independent of  $k_F$ , that is, of the electron density, and depends only on natural constants and the dielectric constant.
- (3) For screened charged impurities the corrections are convergent. For point-like impurities the corrections are convergent in the multilayer case  $|N| \geq 2$  but require an ultraviolet cut-off in the monolayer case  $N = \pm 1$ .
- (4) For point-like impurities in the multilayer case  $|N| \neq 1$  the contribution from principal value terms vanishes trivially to orders  $(\ell k_F)^0$  and  $(\ell k_F)^{-1}$ . The leading quantum correction is then the correction of order  $(\ell k_F)^{-1}$  derived with principal value terms neglected.

The first conclusion is in qualitative agreement with Trushin *et al* [21]. The ac result does not correspond to the frequency dependent correction  $\sim(\ell k_F)^0$  found by Culcer *et al* [22, 35]. The second conclusion appears to disagree with Auslender *et al* [20] who present a leading quantum correction of order  $(\ell k_F)^{-1}$ .<sup>7</sup> The third conclusion is in agreement with all the previous studies. The fourth conclusion is consistent with the recent paper [10].<sup>8</sup> We wish to stress that our electron-density-independent contribution  $\sim(\ell k_F)^0$  to the conductivity has a different origin than those discussed in previous studies [21, 22].

Electron–hole coherent quantum correction gives, with the shift  $(\ell k_F)^0$ , one mechanism for generating a residual conductivity (see figure 1). Our shift could therefore play a part in the residual conductivity observed in the experiments by Chen *et al* [13] on monolayer graphene. This residual conductivity—estimated to be  $2.6e^2/h$ —is observed to be surprisingly constant, depending at most weakly on impurity density, in contrast to the conductivity minimum. Our contribution to the residual conductivity is independent of the impurity density. However, it can in principle depend on the dielectric environment of the graphene sample. There are experiments varying the dielectric constant, for example by coating the sample with ice [36]. However, here the extraction of the residual conductivity appears to be more precarious, and it is too early to say if there is any relation to the dielectric behavior of our contribution.

The second aim of the paper is to compare different derivations of collision integrals for graphene and to extend the repertoire to Green’s function approaches. Double-time

<sup>7</sup> Concerning this disagreement Katsnelson communicated to us that their equations (84) and (85) are not the full results and that the full result treated in the appendix of their paper might also contain contributions of order  $\mathcal{O}(1)$  (see also the statement at the end of their appendix) in which case the qualitative disagreement could be removed.

<sup>8</sup> Conclusion (3) for multilayers is revised in the second version (3) of our preprint thanks to discussions with Trushin. Furthermore, Trushin’s observation of the vanishing of principal value terms for point-like impurities in the bilayer case  $N = 2$  with a density matrix approach prompted us in the second version of the preprint to extract from our general analysis the consequences for the multilayer case  $|N| \geq 2$  with point-like impurities, one of them being conclusion (4).

approaches require, however, the choice of an Ansatz. We will see that different choices lead to qualitatively different general collision integrals. Some of our results are:

- (1) The standard choices of the Kadanoff–Baym Ansatz (KBA) [37] or the generalized Kadanoff–Baym Ansatz (GKBA) [38] do not give the same general collision integral as the single-time density matrix approaches.
- (2) We propose an alternative Ansatz—AA (‘anti-ordered Ansatz’)—for which the translation between density matrix and Green’s function approaches can be established.
- (3) For the symmetrized KB Ansatz (SKBA) given by the sum of GKBA and AA the principal value terms can be completely absent.
- (4) For spinless electrons, and to zeroth order in the gradient expansion, the general collision integrals of all approaches coincide. This applies even in the presence of spin–orbit coupling, provided the latter is small. The difference between collision integrals enters into the principal value terms, which vanish for zero spin–orbit coupling (to zeroth order in the gradient expansion). The difference also enters into the delta function terms, but only in parts that capture second and higher order effects in the spin–orbit interaction.
- (5) Both with and without principal value terms, the leading quantum correction to the graphene Drude conductivity in general depends on the approach. The difference can be quantitative (for example a factor 3 for point-like impurities in the monolayer case  $|N| = 1$  with principal value terms neglected when comparing the result derived with a density matrix approach to the result derived with a Green’s function approach implementing the GKBA) or, when principal value terms are included, even qualitative (of different order in  $(\ell k_F)^{-1}$  or of opposite sign, in the case of point-like impurities in monolayers  $|N| = 1$  of different ultraviolet divergent behavior).

The exception to the last conclusion is the case of point-like impurities in a bilayer  $|N| = 2$ . In this case the principal value terms vanish in all approaches and the remaining delta function terms of the collision integral coincide. Therefore the density matrix approach of [10] is not affected by the ambiguities unraveled in the present paper.

Conclusion (4), also partly discussed in [27], might explain why the difference between a density matrix approach and a Green’s function approach with the GKB Ansatz does not seem to have been an issue for debate<sup>9</sup>, even in similar contexts such as spin-coherent Boltzmann treatments of the spin Hall effect, where there is a greater variety of applied approaches, see [23]–[27]. With the focus on spin and charge currents to leading order, the typical neglect of principal value terms seems acceptable. Furthermore, the energy  $b$  of the spin–orbit coupling is typically assumed to be small compared to the spin-diagonal

<sup>9</sup> It can be interesting to notice that in the field of transport through quantum dots the dichotomy of a density matrix (master equation/superoperator) approach versus a Green’s function approach has been discussed (see Timm [60]) and the question of their equivalence has been raised. There the two approaches are somewhat complementary, the first from the perspective of the dot that gets tunneled through whereas the second is from that of the electron that tunnels. Although there is no firm proof of the equivalence, the general impression seems to be that the approaches should be equivalent since they are both believed to be correct. Therefore, to the extent that the different approaches are believed to be correct also in the context of graphene, the present paper could add some new valuable input to this dichotomy. To our knowledge the issue of Ansatz has not been raised in this context.

part  $\epsilon_0 \sim p^2/2m$  of the kinetic energy to justify an expansion in the collision integrals to first order in  $b_F/\epsilon_{0F}$ , see [24, 26, 27]. The difficulty of solving the Boltzmann equation analytically increases rapidly with higher orders in  $b_F/\epsilon_{0F}$ , and appears to be beyond reach without an expansion. However, in the special case of  $\epsilon_0 = 0$ , the case of graphene, many simplifications occur which enable an analytic solution even for a strong spin-orbit coupling. The circumstance  $\epsilon_0 = 0$  is what allows us to analytically explore the differences in predictions between the different approaches.

Apart from the issue of the principal value terms the common framework of approximations of the related works are adopted in the present paper. In particular we assume a low impurity concentration, restrict ourselves to the lowest order in the Born approximation and neglect weak (anti-)localization corrections. This framework also includes two further approximations:

- (1) Terms involving the interactions (self-energy terms) are taken only to zeroth order in the gradient expansion while the free part of the kinetic equation is expanded to first order in the gradients (in order to recover the driving terms).
- (2) The Wigner transformed density matrix of the electron  $\rho(\mathbf{p}, \mathbf{x}, t) \sim \int d\omega G^<(\mathbf{p}, \omega, \mathbf{x}, t)$  is identified with the Landau quasiparticle distribution function  $f(\mathbf{p}, \mathbf{x}, t)$ . The former is the quantity for which the kinetic equations are formally derived and in terms of which the currents are expressed, the latter is the quantity which in equilibrium is given by a Fermi-Dirac distribution.

Although each one of these approximations seems to be inconsistent at first sight, both are standard. They are perfectly fine for the derivation of a lowest order result like the Drude conductivity or the spin Hall current. These approximations break down as soon as one has to consider quantum corrections due to strong interactions or strong fields beyond linear response. (See [30, 39].) However, it would be far too ambitious at present to also properly account for gradient corrections and the difference between  $\rho$  and  $f$  in our study. Also, such a treatment would not directly be concerned with the two mentioned purposes of our study, but rather with the global goal, namely that of a fully consistent and systematic Boltzmann treatment of the first quantum correction. This problem is work in progress that we hope to return to in the future.

In this paper we have mainly graphene in mind. However, the results apply to any setting in 2d where the electrons are described by one or several independent Dirac cones. Our results should therefore also be relevant for some 3d topological insulators such as  $\text{Bi}_{1-x}\text{Sb}_x$ ,  $\text{Bi}_2\text{Te}_3$ ,  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$  with the 2d surface states described by Dirac electrons [40]–[45], see also [46]. In particular, the occurrence of a single Dirac cone removes the problem of inter-valley scattering. Thus, these systems should be a better application of those of our calculations that deal with point-like impurities, for which we would expect our assumption of negligible inter-valley scattering to be invalid.

The outline of the paper is the following. In section 2 we present the Wigner transformed Hamiltonians that we examine in this paper. In section 3 the semiclassical distribution function and the Boltzmann equation for a spin-orbit coupled system are introduced. Derivations of collision integrals with different approaches are presented in section 4. In section 5 the different general collision integrals are compared and simplified for the case of spin-orbit coupled systems, in particular graphene. Section 6 deals with the solution of the Boltzmann equation neglecting principal value terms and the resulting

dc conductivity. Section 7 contains the ac current generalization thereof. In section 8, we solve the Boltzmann equation including the principal value terms and present the resulting conductivity, both dc and ac. At the beginning of that section we also discuss the physical background of the principal value terms. At the end of that section we discuss whether finite electron-hole coherence effects far away from the Dirac point make sense. Conclusions and an outlook are given in section 9.

## 2. The model

For a semiclassical Boltzmann description (see e.g. [39], [47]–[49]) one typically uses the Wigner transformed one-particle Hamiltonian. For the spin-orbit coupled systems that we set out to study, the Hamiltonian in the absence of impurities reads

$$H(\mathbf{x}, \mathbf{p}, t) = \epsilon_0(k) + \boldsymbol{\sigma} \cdot \mathbf{b}(\mathbf{k}) + e\phi(\mathbf{x}, t) \quad (1)$$

with  $e < 0$  and  $\mathbf{k}(\mathbf{x}, \mathbf{p}, t) = \mathbf{p} - e\mathbf{A}(\mathbf{x}, t)$ . The energy bands in the absence of electromagnetic fields are  $\epsilon_{\mathbf{k}}^s = \epsilon_0 + sb$ , with  $s = \pm$  giving the sign of the spin along the spin quantization axis  $\hat{\mathbf{b}}$ , i.e.  $\boldsymbol{\sigma} \cdot \hat{\mathbf{b}}|\hat{\mathbf{b}}_s\rangle = s|\hat{\mathbf{b}}_s\rangle$ . We want to describe a 2d system with  $\mathbf{x}$  and  $\mathbf{p}$  chosen to lie in the  $x, y$ -plane. We set  $\hbar = 1$ .

The spinless part of the dispersion is given by  $\epsilon_0$ . In the spin-orbit coupled systems studied in the intrinsic spin Hall effect, this is typically the quadratic dispersion  $\epsilon_0 = k^2/2m^*$ , and usually constitutes the greater part of the kinetic energy. For monolayer graphene, the spin-orbit coupling entirely constitutes the kinetic part, i.e.  $\epsilon_0 = 0$ . The spin here is the pseudospin given by the bipartite lattice. Additionally, the electrons have a valley index corresponding to the two Dirac cones, K and K', as well as the real spin index. The real spin index will be treated as trivial in the present paper. Furthermore, we will neglect inter-valley scattering in order to treat each Dirac cone independently and therefore deal only with the  $2 \times 2$  Hamiltonian (1). This approximation should be fine if the disorder is smooth but should break down if the impurity potential is too short-ranged, as in the extreme case of point-like impurities.

For the Dirac point K the spin-orbit coupling for the pseudospin is given by  $\mathbf{b} = v_F \mathbf{k}$  (i.e.  $b = v_F k$  and  $\hat{\mathbf{b}} = \hat{\mathbf{k}}$ ) with  $v_F \approx c/300$  being the Fermi velocity. We consider the more general isotropic spin-orbit coupling  $\mathbf{b} = b(k)\hat{\mathbf{b}}(\theta)$  with a winding number  $N$  given by  $\hat{b}_x + i\hat{b}_y = e^{i\theta_0 + iN\theta}$  ( $\theta_0$  is a constant). This includes the Dirac cone K' ( $b = v_F k$  and  $\hat{\mathbf{b}} = (\cos \theta, -\sin \theta)$ , i.e.  $N = -1$ ) of monolayer graphene and the Hamiltonian

$$H = \frac{1}{2m^*} \begin{pmatrix} 0 & (k_x \mp ik_y)^2 \\ (k_x \pm ik_y)^2 & 0 \end{pmatrix} = \frac{k^2}{2m^*} \begin{pmatrix} 0 & e^{\mp i2\theta} \\ e^{\pm i2\theta} & 0 \end{pmatrix} \quad (2)$$

( $b = k^2/2m^*$  and  $N = 2$ ) studied in the context of bilayer graphene as well as similar Hamiltonians studied in multilayer graphene [31]–[34].

The total Hamiltonian  $H_{\text{tot}} = H + V$  includes an impurity potential  $V(\mathbf{x}) = \sum_n u(\mathbf{x} - \mathbf{x}_n)$  of non-magnetic impurities at positions  $\mathbf{x}_n$  eventually to be averaged over. We distinguish between point-like impurities  $u_{\mathbf{k}\mathbf{k}'} = \text{const.}$  and screened charged impurities in 2d with

$$u_{\mathbf{k}\mathbf{k}'} = \frac{e^2/\kappa_d}{|\mathbf{k} - \mathbf{k}'| + k_{\text{TF}}} \quad (3)$$

with the Thomas–Fermi momentum  $k_{\text{TF}} = (2\pi e^2/\kappa_{\text{d}})D(\epsilon_{\text{F}})$  giving the range  $L_s = 1/k_{\text{TF}}$  of the screened potential.  $\kappa_{\text{d}}$  is the dielectric constant. For a recent review on screening in graphene with an enlightening comparison of monolayers with bilayers and 2DEGs, see [50]. Here we will recollect a few facts that will be important for our later discussions.

It is convenient to introduce the dimensionless parameter  $q_s := k_{\text{TF}}/k_{\text{F}}$  characterizing the strength of the screening. An unscreened Coulomb interaction corresponds to  $q_s = 0$ . In the opposite limit  $q_s \rightarrow \infty$  the potential becomes almost angularly independent and behaves in some respects as a point-like impurity, although not in all aspects. In the monolayer case, for example, one has the unique situation that  $D_{\text{F}} \propto k_{\text{F}}$ , hence  $q_s$  is independent of  $k_{\text{F}}$ , implying that for both short and long screening lengths the potential behaves as an unscreened Coulomb potential in that  $\tau_{\text{tr}}^{-1}(k_{\text{F}}) \propto D_{\text{F}}k_{\text{F}}^{-2} \propto k_{\text{F}}^{-1}$  and therefore  $\sigma_0 \sim \tau_{\text{tr}}(k_{\text{F}})\epsilon_{\text{F}} \propto k_{\text{F}}^2 \propto |n|$ . Thus, not even with strong screening does the situation turn into that of point-like impurities, where  $\tau_{\text{tr}}^{-1} \propto k_{\text{F}}$  predicts a Drude conductivity independent of density. For graphene on  $\text{SiO}_2$  substrates, the standard value is

$$q_s \approx 3.2. \quad (4)$$

This suggests that screening is important ( $q_s > 1$ ) and when discussing the quantum correction  $(\ell k_{\text{F}})^0$  we will argue that this correction for the screened potential with the given  $q_s$  is nonetheless more closely related to the results for point-like impurities than to those of an unscreened Coulomb potential.

In bilayers and multilayers the situation is very different. Here  $q_s$  decreases with  $k_{\text{F}}$ , and consequently with the density, just like in an ordinary 2DEG, but opposite to a 3DEG. Thus, the further we move away from the Dirac point, the weaker the screening and the stronger the effect of the interaction. Thus, when discussing the correction  $(\ell k_{\text{F}})^0$  we expect that in the vicinity of the Dirac point the screened potential has more in common with point-like impurities, whereas far away from the Dirac point the potential has more in common with an unscreened Coulomb potential.

### 3. Semiclassical description of a spin–orbit coupled system

In a Boltzmann picture the spatial degrees of freedom can be treated semiclassically. The treatment of the pseudospin must, on the contrary, remain quantum mechanical in order to capture electron–hole coherence effects. The state of the system is described by the Wigner transform  $\rho_{\sigma\sigma'}(\mathbf{x}, \mathbf{p}, t)$  of the time-diagonal density matrix

$$\rho_{\sigma\sigma'}(x_1, x_2, t_1) = \langle \Psi_{\sigma'}^\dagger(\mathbf{x}_2, t_1) \Psi_\sigma(\mathbf{x}_1, t_1) \rangle = G_{\sigma\sigma'}^<(x_1, t_1, x_2, t_2)_{t_2=t_1} \quad (5)$$

for electrons with spin indices  $\sigma = \uparrow_z, \downarrow_z$ . (See e.g. [39], [47]–[49].) In the absence of interactions one can derive a Boltzmann equation for  $\rho$  by applying the Heisenberg equation of motion on  $\Psi(t_1)$ , then identifying  $t_2 = t_1$ , Wigner transforming the result, and gradient expanding to first order. The approximation to stop at the first order in the gradient expansion is the *semiclassical* approximation, which assumes that the external perturbations, such as electromagnetic potentials, change negligibly on length and time scales of the de Broglie wavelength  $\lambda_{\text{B}}$  and the time  $\tau_{\text{B}} = \lambda_{\text{B}}/v_{\text{F}}$ . Upon Wigner transformation  $X(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) \rightarrow X(\mathbf{x}, \mathbf{p}, t, \omega)$  (for the time-diagonal approaches the Wigner transformation only involves the spatial part, not time) the convolution product is translated into  $XY \rightarrow X e^{(i/2)\mathcal{D}} Y$ , where the matrix product in spin remains but the

convolution of time and real space variables is replaced by a Moyal product with a Poisson-bracket-like gradient  $\mathcal{D}$ . In a gauge invariant treatment, valid when the electromagnetic fields are weak and vary slowly (see e.g. [47]), one introduces  $\mathbf{k}(\mathbf{p}, \mathbf{x}, t) = \mathbf{p} - e\mathbf{A}$  and  $\tilde{\omega}(\omega, \mathbf{x}, t) = \omega - e\phi$  and lets  $\{\mathbf{x}, \mathbf{k}, t, \tilde{\omega}\}$  become the new set of independent variables (i.e.  $\partial_{x_i}\mathbf{k} = 0$ ). This changes the gradient into

$$\mathcal{D} = \overleftarrow{\partial}_{x_i} \overrightarrow{\partial}_{k_i} - \overleftarrow{\partial}_{k_i} \overrightarrow{\partial}_{x_i} + \overleftarrow{\partial}_{\tilde{\omega}} \overrightarrow{\partial}_t - \overleftarrow{\partial}_t \overrightarrow{\partial}_{\tilde{\omega}} + E_i(\overleftarrow{\partial}_{\tilde{\omega}} \overrightarrow{\partial}_{k_i} - \overleftarrow{\partial}_{k_i} \overrightarrow{\partial}_{\tilde{\omega}}) + \epsilon_{ijl} B_i \overleftarrow{\partial}_{k_j} \overrightarrow{\partial}_{k_l} \quad (6)$$

with  $X \overleftarrow{\partial} Y := (\partial X)Y$  and  $X \overrightarrow{\partial} Y := X(\partial Y)$ .

From the matrix elements of the distribution function  $\rho$ , one extracts the densities and current densities of charge and spin. The matrix elements are conveniently expressed in the decomposition  $\rho = \rho_0 + \boldsymbol{\sigma} \cdot \boldsymbol{\rho}$ , where  $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  is the vector of Pauli matrices. Furthermore, we find it convenient to decompose the vector  $\boldsymbol{\rho} = \rho_{\hat{\mathbf{b}}} \hat{\mathbf{b}} + \rho_{\hat{\mathbf{c}}} \hat{\mathbf{c}} + \rho_z \hat{\mathbf{z}}$  into its components along the basis vectors  $\hat{\mathbf{b}}(\theta)$ ,  $\hat{\mathbf{z}}$  and  $\hat{\mathbf{c}}(\theta) = \hat{\mathbf{z}} \times \hat{\mathbf{b}}(\theta)$  with  $\partial_\theta \hat{\mathbf{b}} = N\hat{\mathbf{c}}$ , analogous to the cylindrical basis vectors  $\hat{\mathbf{k}}(\theta) := \mathbf{k}/k$ ,  $\hat{\mathbf{z}}$  and  $\hat{\boldsymbol{\theta}}(\theta) := \hat{\mathbf{z}} \times \hat{\mathbf{k}}(\theta)$  with  $\partial_\theta \hat{\mathbf{k}} = \hat{\boldsymbol{\theta}}$ . In the spin basis  $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$  one has

$$\rho = \rho_0 \mathbf{1} + \rho_{\hat{\mathbf{b}}} \hat{\mathbf{b}} \cdot \boldsymbol{\sigma} + \rho_{\hat{\mathbf{c}}} \hat{\mathbf{c}} \cdot \boldsymbol{\sigma} + \rho_z \hat{\mathbf{z}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} \rho_0 + \rho_z & (\rho_{\hat{\mathbf{b}}} - i\rho_{\hat{\mathbf{c}}})e^{-iN\theta} \\ (\rho_{\hat{\mathbf{b}}} + i\rho_{\hat{\mathbf{c}}})e^{iN\theta} & \rho_0 - \rho_z \end{pmatrix}. \quad (7)$$

The charge density  $en$  and current density  $e\mathbf{j}$  in phase space are derived from  $en = \text{Tr}(\rho \partial H / \partial \phi)$  and  $e\mathbf{j} = -\text{Tr}(\rho \partial H / \partial \mathbf{A})$ , which yields

$$n(\mathbf{x}, \mathbf{k}, t) := \text{Tr} \rho = 2\rho_0 = n^+ + n^-, \quad (8)$$

$$j_i(\mathbf{x}, \mathbf{k}, t) := \text{Tr}(\mathbf{v}_i \rho) = 2\rho_0 \partial_{k_i} \epsilon_0 + 2\boldsymbol{\rho} \cdot \partial_{k_i} \mathbf{b} = n^+ v_i^+ + n^- v_i^- + \frac{2Nb}{k} \rho_{\hat{\mathbf{c}}} \hat{\theta}_i$$

with  $i = x, y$ . Here we introduced the velocity matrices  $\mathbf{v}_i := \partial_{k_i} H = \partial_{k_i} \epsilon_0 + \boldsymbol{\sigma} \cdot \partial_{k_i} \mathbf{b}$ . The spin independent part of the velocity is  $\partial_{\mathbf{k}} \epsilon_0 =: \mathbf{v}_0$ . The band velocities are  $\mathbf{v}^s := \partial_{\mathbf{k}} \epsilon^s = \langle \hat{\mathbf{b}}^s | \mathbf{v} | \hat{\mathbf{b}}^s \rangle = v^s \hat{\mathbf{k}}$ . The *intra*-band elements

$$n^\pm := \langle \hat{\mathbf{b}}^\pm | \rho | \hat{\mathbf{b}}^\pm \rangle = \rho_0 \pm \rho_{\hat{\mathbf{b}}} \quad (9)$$

give the density in each spin band  $s = \pm$ . The *inter*-band elements  $\langle \hat{\mathbf{b}}^\pm | \rho | \hat{\mathbf{b}}^\mp \rangle = \rho_z \pm i\rho_{\hat{\mathbf{c}}}$  are important for the coherent treatment of spin. These are the elements that oscillate in the occurrence of spin-precession. In the case of spin-orbit coupling the imaginary component  $\rho_{\hat{\mathbf{c}}}$  appears in the last term of the current (8).<sup>10</sup> For the density matrix of a single electron this term would contain the oscillatory Zitterbewegung motion of the free spin-orbit coupled electron. In the statistical description given by the distribution function this oscillatory motion of the free particle states averages to zero over time and is therefore absent in the equilibrium distribution function ( $\rho_{\hat{\mathbf{c}}}^{\text{eq}} = \rho_z^{\text{eq}} = 0$ ).

Throughout the paper we write the Boltzmann equation and the distribution function in the momentum independent spin basis  $\{|\uparrow_z\rangle, |\downarrow_z\rangle\}$ . Some studies (e.g. [20, 21]) prefer to transform the Boltzmann equation into the momentum dependent eigenbasis  $\{|\hat{\mathbf{b}}^+\rangle, |\hat{\mathbf{b}}^-\rangle\}$ . For example, the velocity matrix for graphene ( $\epsilon_0 = 0$ )

$$\mathbf{v} = \sigma_i \left( \hat{\mathbf{k}} \partial_k + \frac{1}{k} \hat{\boldsymbol{\theta}} \partial_\theta \right) b_i = \hat{\mathbf{k}} \boldsymbol{\sigma} \cdot \hat{\mathbf{b}} \partial_k b + \hat{\boldsymbol{\theta}} \boldsymbol{\sigma} \cdot \hat{\mathbf{c}} \frac{Nb}{k} = \begin{pmatrix} \hat{\mathbf{k}} \partial_k b & i\hat{\boldsymbol{\theta}} \frac{Nb}{k} \\ -i\hat{\boldsymbol{\theta}} \frac{Nb}{k} & -\hat{\mathbf{k}} \partial_k b \end{pmatrix}^{\text{ch}} \quad (10)$$

<sup>10</sup> Note also that this term is equally shared between the two bands;  $\langle \hat{\mathbf{b}}^s | \frac{1}{2} \{ \mathbf{v}, \rho \} | \hat{\mathbf{b}}^s \rangle = n^s \mathbf{v}^s + k^{-1} b \rho_{\hat{\mathbf{c}}} \hat{\boldsymbol{\theta}}$ .

when written in the latter basis (the superscript ‘ch’ indicating the chirality/helicity basis). For the distribution function the relation is

$$\begin{aligned}\rho &= \rho_0 \mathbf{1} + \rho_{\hat{\mathbf{b}}} \hat{\mathbf{b}} \cdot \boldsymbol{\sigma} + \rho_{\hat{\mathbf{c}}} \hat{\mathbf{c}} \cdot \boldsymbol{\sigma} + \rho_z \hat{\mathbf{z}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} \rho_0 + \rho_{\hat{\mathbf{b}}} & \rho_z + i\rho_{\hat{\mathbf{c}}} \\ \rho_z - i\rho_{\hat{\mathbf{c}}} & \rho_0 - \rho_{\hat{\mathbf{b}}} \end{pmatrix}^{\text{ch}} \\ &= \rho_0 \mathbf{1} + \rho_{\hat{\mathbf{b}}} \sigma_z^{\text{ch}} - \rho_{\hat{\mathbf{c}}} \sigma_y^{\text{ch}} + \rho_z \sigma_x^{\text{ch}}.\end{aligned}\quad (11)$$

The Pauli matrices  $\sigma_i^{\text{ch}}$  have nonzero momentum derivatives ( $\partial_\theta \sigma_z^{\text{ch}} = -N \sigma_y^{\text{ch}}$ ,  $\partial_\theta \sigma_y^{\text{ch}} = N \sigma_z^{\text{ch}}$  and  $\partial_\theta \sigma_x^{\text{ch}} = 0$ ). The eigenbasis has the attractive feature of allowing one to identify the intra-band densities  $n^\pm = \rho_0 \pm \rho_{\hat{\mathbf{b}}}$  as the diagonal matrix elements. However, this would not be of any advantage in our treatment of graphene, where we only need the spin components and need to distinguish between  $\rho_{\hat{\mathbf{b}}}$ ,  $\rho_{\hat{\mathbf{c}}}$  and  $\rho_z$  rather than to view the problem in terms of  $\rho_{+-}(=\rho_{-+}^*)$ ,  $\rho_{++}(=n^+)$  and  $\rho_{--}(=n^-)$ . The charge component  $\rho_0$  will in our problem be redundant and completely decoupled.

The spin density, i.e. the polarization, is given by  $s^\mu = \frac{1}{2} \text{Tr}(\sigma_\mu f) = \rho_\mu$  (with  $\mu = x, y, z$ ). There is no unique way to define the spin current because, in presence of spin-orbit coupling, the real space spin polarization is not a conserved quantity. When band velocities coincide ( $\mathbf{v}^s = \mathbf{v}_0$ ) it is  $\mathbf{j}^\mu = \rho_\mu \mathbf{v}_0$ . A common definition is

$$j_i^\mu = \frac{1}{4} \text{Tr} \sigma_\mu \{ \mathbf{v}_i, \rho \} = \rho_\mu \partial_{k_i} \epsilon_0 + \rho_0 \partial_{k_i} b_\mu \quad (12)$$

(with  $\{A, B\} = AB + BA$ ). Notice that in the graphene case  $\epsilon_0 = 0$  one is confronted with the peculiar situation that the charge current is only determined by the spin density, whereas the spin current is only determined by the charge density. Here one should remember that it is electrons and *holes* that contribute additively to the current. The current is therefore determined by the charge carrier density, that is by the sum of the densities of electrons ( $n^+$ ) and holes ( $1 - n^-$ )—i.e. by  $n^+ + (1 - n^-) = 1 + 2\rho_{\hat{\mathbf{b}}}$ —rather than by the difference  $n^+ - (1 - n^-) = -1 + 2\rho_0$ . In the presence of a magnetic field one needs to involve  $\rho_0$ . In the Hall component of the conductivity it is the difference of electrons and holes that contributes.

The Boltzmann equation in matrix form is given by

$$i[H, f] + \partial_t \rho + \frac{1}{2} \{ \mathbf{v}_i, \partial_{x_i} \rho \} + e E_i \partial_{k_i} \rho - \epsilon_{zij} e B_z \frac{1}{2} \{ \mathbf{v}_i, \partial_{k_j} \rho \} = \mathcal{J}[\rho] \quad (13)$$

where the matrix-valued functional  $\mathcal{J}$  is the collision integral. With the definition (12) the Boltzmann equation (13) can be written in the appealing form

$$\begin{aligned}\partial_t n + \partial_x \cdot \mathbf{j} + e \partial_k \cdot (n \mathbf{E} + \mathbf{j} \times \mathbf{B}) &= 2\mathcal{J}_0, \\ 2(\mathbf{s} \times \mathbf{b})^\mu + \partial_t s^\mu + \partial_x \cdot \mathbf{j}^\mu + e \partial_k \cdot (s^\mu \mathbf{E} + \mathbf{j}^\mu \times \mathbf{B}) &= \mathcal{J}_\mu.\end{aligned}\quad (14)$$

Semiclassical kinetic equations deal as above with densities in phase space. Densities in real space are obtained by integrating the phase space densities over momentum, e.g.

$$\mathbf{j}(\mathbf{x}, t) = \int \frac{d^2 k}{(2\pi)^2} \mathbf{j}(\mathbf{x}, \mathbf{k}, t). \quad (15)$$

The Boltzmann equation is typically written in terms of the quasiparticle distribution  $f_{\sigma\sigma'}(\mathbf{x}, \mathbf{p}, t)$  rather than in terms of the Wigner transformed density matrix  $\rho_{\sigma\sigma'}(\mathbf{x}, \mathbf{p}, t)$ . The electron distribution  $\rho$  is the quantity in terms of which the current and densities are defined. The quasiparticles described by  $f$  on the other hand represent the free particles

that satisfy the Pauli principle. Thanks to this the equilibrium state can, for  $f$ , be expressed simply in terms of the Fermi–Dirac distribution. This is of practical relevance in the analytical solving of the Boltzmann equation by linearizing around equilibrium. In this paper we neglect this difference. Thus, all expressions including  $\rho$  are assumed to apply for  $f$ .

#### 4. Derivation of collision integrals

The presence of, for example, electron–electron interactions, phonons or impurities, is captured in the collision integral  $\mathcal{J}$ . It is assumed that one is in the *kinetic regime*, where the de Broglie wavelength  $\lambda_B = 1/k_F$  is much shorter than the scattering length  $\ell$ , which translates into  $\ell k_F \ll 1$ . We will only deal with averaged non-magnetic impurities. The averaging over of impurity positions in  $V_{kk'} = \sum_n e^{-i(k-k')x_n} u_{kk'}$  restores the translational invariance<sup>11</sup>.

In this section we will go through some of the possible approaches for the derivation of semiclassical kinetic equations including collision integrals from quantum theory. One group of approaches deals directly with the density matrix  $\rho(x_1, x_2, t)$  and starts from the von Neumann (quantum Liouville) equation  $i\partial_t \rho = [H, \rho]$ . The second group of approaches are Green’s function techniques which have the Kadanoff–Baym or Keldysh equations for the double-time correlator  $G^<(x_1, t_1, x_2, t_2)$  as their starting points. To recover a time-diagonal kinetic equation in the latter requires some approximation. This is the problem of the Ansatz. We will see several different candidates and therefore several different collision integrals. One of them is identical to the collision integral derived with the density matrix approaches.

##### 4.1. Iterative solution of the von Neumann equation (quantum Liouville equation)

The simplest derivation of a collision integral is probably one in which the von Neumann equation is iterated to second order in the interaction. Let  $H_{\text{tot}} = H_0 + V$ , where  $V$  is an interaction switched on at a time  $t_0$  in the remote past. The von Neumann equation in the interaction picture is

$$i\partial_t \rho^I = [V^I(t), \rho^I] \quad (16)$$

with  $A^I(t) = e^{iH_0 t} A(0) e^{-iH_0 t} = \mathcal{U}_0^\dagger(t) A(0) \mathcal{U}_0(t)$ . This is easily integrated to give

$$\rho^I(t) = \rho^I(t_0) - i \int_{t_0}^t dt' [V^I(t'), \rho^I(t')] \quad (17)$$

which, when inserted back into (16), yields

$$\begin{aligned} \partial_t \rho^I &= -i[V^I(t), \rho^I(t_0)] - \int_{t_0}^t dt' [V^I(t), [V^I(t'), \rho^I(t')]] \\ &= -i[V^I(t), \rho^I(t_0)] - \int_{t_0}^t dt' [V^I(t), [V^I(t'), \rho^I(t')]] \\ &\quad - i \int_{t_0}^t \int_{t'}^t dt'' [V^I(t), [V^I(t'), [V^I(t''), \rho^I(t'')]]] \end{aligned} \quad (18)$$

<sup>11</sup> The averaging implies  $V_q \rightarrow n_{\text{imp}} V_q \delta(q) \sim n_{\text{imp}} V(r = 0)$  and  $\dots V_{q_1} \dots V_{q_2} \dots \rightarrow (\dots V_{q_1} \dots V_{q_2} \dots) [n_{\text{imp}}^2 \delta(q_1) \delta(q_2) + n_{\text{imp}} \delta(q_1 + q_2)]$ . For the last term we neglect the  $n_{\text{imp}}^2$  through the assumption of low impurity concentration.

after a first and second iteration, respectively. So far the equations are exact. The Born approximation allows us to get a closed equation for  $\rho$  at time  $t$  to second order in the interaction  $V$ . To this end we remove the last term in the third row. Alternatively, in the last term of the first row replace the full evolution with the free evolution, i.e. let  $\rho^I(t') = \rho^I(t)$ , which has the appearance of a Markov approximation. Back in the Schrödinger picture the assumption of free evolution reads

$$\rho(t') = \mathcal{U}_0(t', t) \rho(t) \mathcal{U}_0^\dagger(t', t) = e^{-iH_0(t', t)} \rho(t) e^{iH_0(t', t)} \quad (19)$$

and after reorganizing evolution operators one obtains the kinetic equation in the Schrödinger picture,

$$\partial_t \rho(t) - i[H_0, \rho(t)] = -i[V, e^{-H_0(t-t_0)} \rho(t_0) e^{iH_0(t-t_0)}] - \int_0^{t-t_0} d\tau [V, [e^{-iH_0\tau} V e^{iH_0\tau}, \rho(t)]] \quad (20)$$

So far, this kinetic equation is locally time reversible (not globally though, since we switched on the interaction). To capture the decoherence due to other processes (phonons etc) we do not want the state to depend on correlations in the remote past. Therefore we include a factor  $e^{-\eta\tau}$  in the integral to impose this loss of memory. This introduces time irreversibility. This factor also regularizes the integral and allows us to send  $t_0 \rightarrow -\infty$ . In translating the evolution operators into Green's functions (see appendix A), the last term can be written as

$$\mathcal{J}[\rho] = - \int \frac{d\omega}{2\pi} [V, [G^{0R} V G^{0A}, \rho]], \quad (21)$$

where we anticipated that the last term will become the collision integral  $\mathcal{J}$ .

Another source of irreversibility comes with the impurity averaging procedure, a coarse graining that also captures the decoherence due to phonons, for example. Then  $V$  in the first term becomes just a number  $\sim V(r=0)$  and the commutator vanishes<sup>12</sup>. For the terms linear in  $n_{\text{imp}}$  one finds for example (summation over repeated indices implicit)

$$(V G^{0R} V G^{0A} \rho)_{kk'} \longrightarrow n_{\text{imp}} \delta(k - k_1 + k_1 - k_2) u_{kk_1} G_{k_1}^{0R} u_{k_1 k_2} G_{k_2}^{0A} \rho_{k_2 k'} = \Sigma_k^R G_k^{0A} \rho_{kk'}, \quad (22)$$

where we introduced the retarded self-energy  $\Sigma_k^R = n_{\text{imp}} (u G^{0R} u)_k$ . However, in a term like

$$(V \rho G^{0R} V G^{0A})_{kk'} \longrightarrow n_{\text{imp}} \delta(k - k_1 + k_2 - k') u_{kk_1} \rho_{k_1 k_2} G_{k_2}^{0R} u_{k_2 k'} G_{k'}^{0A} \quad (23)$$

the delta function seems to offer no simplification at all.

At this point we can attain further simplification if we say that in the collision integral we are not interested in any contributions which have to do with non-diagonality in momentum. This actually amounts to saying that we are not interested in any gradient expansion corrections to the collision integral:

$$(V \rho G^{0R} V G^{0A})_{kk} \longrightarrow n_{\text{imp}} u_{kk'} \rho_{k'} G_{k'}^{0R} u_{k'k} G_k^{0A}. \quad (24)$$

<sup>12</sup> In the derivation of master equations for quantum dots this term vanishes for another reason, see e.g. [60]. For  $t \leq t_0$  the state is a simple product state  $\rho = \rho_{\text{dot}} \otimes \rho_{\text{lead}}^{\text{eq}}$  with the leads assumed to be in equilibrium. Since  $\rho_{\text{lead}}^{\text{eq}}$  has a definite particle number whereas the hopping interaction  $V$  changes the particle number, tracing over the leads kills this term.

The collision integral can then be written as

$$\mathcal{J}[\rho(\mathbf{k}, \mathbf{x}, t)] = - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \int \frac{d\omega}{(2\pi)^2} (\rho_{\mathbf{k}} G_{\mathbf{k}}^{0R} G_{\mathbf{k}'}^{0A} + G_{\mathbf{k}'}^{0R} G_{\mathbf{k}}^{0A} \rho_{\mathbf{k}} - \rho_{\mathbf{k}'} G_{\mathbf{k}'}^{0R} G_{\mathbf{k}}^{0A} - G_{\mathbf{k}}^{0R} G_{\mathbf{k}'}^{0A} \rho_{\mathbf{k}'}) \quad (25)$$

with the transition matrix  $W_{\mathbf{k}\mathbf{k}'} = 2\pi n_{\text{imp}} |u_{\mathbf{k}\mathbf{k}'}|^2$  for spinless impurities.

A quantum Liouville approach was also used by Culcer *et al* [22], although along different lines. The focus in that treatment was, from the start, only the diagonal part  $f_{\mathbf{k}}$  (not to be confused with our  $f$  for the quasiparticle distribution) of  $\rho_{\mathbf{k}\mathbf{k}'} = f_{\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'} + g_{\mathbf{k}\mathbf{k}'}$ , closing the door to gradient expansion corrections in the interaction terms. The analog of the iterative solution of the Liouville equation in this section is their decomposition into two coupled equations for  $f_{\mathbf{k}}$  and for the purely non-diagonal part  $g_{\mathbf{k}\mathbf{k}'}$ , the integrated equation of the latter then being inserted into the former. Up to this point the approaches are equivalent. The difference comes with the Markov approximation. Culcer *et al* use  $f(t') \rightarrow f(t)$  as opposed to  $f^I(t') \rightarrow f^I(t)$ . With  $\rho(t') \rightarrow \rho(t)$  we find that the evolution operators cancel each other out in a different way so that at the end they sit around the entire inner commutator rather than only around the inner  $V$ ,

$$\mathcal{J}[\rho] = - \int \frac{d\omega}{2\pi} [V, G^{0R}[V, \rho] G^{0A}]. \quad (26)$$

This is indeed the result in equation (4b) in [22]. We will see that the difference between (21) and (26) matters for the first quantum correction. We will also understand why it does not matter for the treatment of [22]. Their recursive analysis taken to order  $(\ell k_{\text{F}})^0$  only requires the part that is insensitive to the differences between (21) and (26).

#### 4.2. Nonequilibrium statistical operator approach

The nonequilibrium statistical operator approach (NSO) [47] is a full-fledged second quantized field theoretical formalism and involves more conceptual and technical ingredients from statistical physics than the approach of section 4.1. It was used in [20] for the derivation of a pseudospin-coherent collision integral for graphene. Like the Green's function formalism, the NSO formalism allows for Wick decompositions and therefore goes beyond the approach of section 4.1 for non-quadratic interactions. For quadratic interactions such as impurities the approaches should be equivalent.

The starting point is again the Liouville equation

$$i\partial_t \hat{\rho}(t) - [H_{\text{tot}}, \hat{\rho}(t)] = -\eta(\hat{\rho}(t) - \hat{\rho}_{\text{rel}}(t)), \quad (27)$$

where  $H_{\text{tot}}$  in contrast to section 4.1 is the second quantized Hamiltonian.  $\eta$  is a small number. The state variable  $\hat{\rho}$  is the *statistical operator*. The density matrix is obtained as the expectation value of the *relevant operators*  $P_m$  ( $m$  is a composite index). In particular, with  $P_{\mathbf{p}\sigma, \mathbf{p}'\sigma'} = c_{\mathbf{p}'\sigma'}^\dagger c_{\mathbf{p}\sigma}$  we have

$$\rho_{\mathbf{k}'}^{\sigma\sigma'} = \langle P_{\mathbf{p}\sigma, \mathbf{p}'\sigma'} \rangle := \text{Tr}(\hat{\rho} P_{\mathbf{p}\sigma, \mathbf{p}'\sigma'}). \quad (28)$$

The novel ingredient on the right-hand side of (27) is included ad hoc to implement the irreversibility already on a fundamental level in the derivation of kinetic equations (thus well before the impurity averaging step in section 4.1). This is done by introducing

an auxiliary statistical operator  $\hat{\rho}_{\text{rel}}$ —the *relevant distribution*—that is the statistical operator with maximal entropy (and therefore minimal quantum mechanical correlations) among all operators with same expectation values for the relevant observables  $P_m$  ( $m$  is a composite index)

$$\langle P_m \rangle_{\text{rel}} := \text{Tr}(\hat{\rho}_{\text{rel}} P_m) = \text{Tr}(\hat{\rho}_{\text{rel}} P_m). \quad (29)$$

The relevant distribution  $\hat{\rho}_{\text{rel}}$  does not evolve according to a Liouville equation like (27) but is determined by the macroscopic observable  $\langle P_m \rangle_t$ . It serves also as an initial condition  $\hat{\rho}(t) = e^{-i(t-t_0)L} \hat{\rho}_{\text{rel}}(t_0)$ , where  $L\rho := [H_{\text{tot}}, \rho]$ . This evolution is however replaced by a coarse grained one,

$$\hat{\rho}(t) = \frac{1}{t-t_0} \int_{t_0}^t dt_i e^{-i(t-t_i)L} \hat{\rho}_{\text{rel}} t_i, \quad (30)$$

(eventually  $t_0 \rightarrow -\infty$ ) to reflect that a macroscopic system forgets the microscopic details of its initial state after some microscopic time. After some more steps for which we refer to the books by Zubarev *et al* [47] one arrives at a general kinetic equation, here to second order in the interaction,

$$\frac{\partial \langle P_m \rangle}{\partial t} + \dots = \mathcal{J}_m(t) = \mathcal{J}_m^{(1)}(t) + \mathcal{J}_m^{(2)}(t) + \mathcal{O}(V^3). \quad (31)$$

The first term of order  $V^1$  is the mean-field contribution

$$\mathcal{J}_m^{(1)}(t) = -i \langle [P_m, V] \rangle_{\text{rel}}^t = -\text{Tr}(\rho_{\text{rel}}(t) [P_m, V]). \quad (32)$$

The second term is of order  $V^2$ ,

$$\mathcal{J}_m^{(2)}(t) := - \int_{-\infty}^t dt' e^{\eta(t'-t)} \text{Tr} \left( \rho_{\text{rel}}(t') \left[ V, \mathcal{U}_0^\dagger(t, t') [V, P_m] \mathcal{U}_0(t, t') + i \sum_n P_n \frac{\delta J_m^{(1)}(t, t')}{\delta \langle P_n \rangle^{t'}} \right] \right). \quad (33)$$

The first term is the familiar double commutator with the interaction. Notice that the average is taken with respect to the relevant statistical distribution, which allows for Wick decomposition (see [47]). For a two-body interaction one will find that the second half, the term with  $\mathcal{J}^{(1)}$ , does not contribute to the collision integral but cancels some anomalous terms from the first half. For impurities,  $\mathcal{J}^{(1)}$  vanishes after impurity averaging. Together with the Born approximation (Markov approximation)

$$\hat{\rho}_{\text{rel}}(t') = \mathcal{U}_0(t', t) \hat{\rho}_{\text{rel}}(t) \mathcal{U}_0^\dagger(t', t) + \mathcal{O}(V) \quad (34)$$

which replaces the full evolution by the free evolution one arrives at ( $\mathcal{U}_0$ , shorthand for  $\mathcal{U}_0(t, t')$ )

$$\begin{aligned} \mathcal{J}_m^{(2)}(t)[\rho] &= - \int_{-\infty}^t dt' e^{\eta(t'-t)} \text{Tr} \left( \mathcal{U}_0^\dagger \rho_{\text{rel}}(t) \mathcal{U}_0 \left[ V, \mathcal{U}_0^\dagger [V, P_m] \mathcal{U}_0 \right] \right) \\ &= - \int_{-\infty}^t dt' e^{\eta(t'-t)} \text{Tr} \left( \rho_{\text{rel}}(t) \left[ \mathcal{U}_0 V \mathcal{U}_0^\dagger, [V, P_m] \right] \right) \\ &= - \int \frac{d\omega}{2\pi} [G^{0R} V G^{0A}, [V, \rho]]. \end{aligned} \quad (35)$$

Notice that this is different from both (21) and (26). We will see that when the collision integrals for graphene is written out explicitly in spin components the result (21) and the result (35) will coalesce.

We would like to mention that [47] also treats the *Cluster expansion method*, which is advantageous compared to NSO for going to higher order in the interaction (deriving the full  $T$ -matrix), whereas NSO has an advantage for dense quantum systems (for deriving two-body collision integrals including the Pauli blocking factors). To second order in the electron–impurity interaction and to linear order in distribution functions both should apply equally. Nonetheless, the collision integral equation (4.2.92) of [47] is not equivalent to (21) or (35) but to the result (26). However, there is again a Markov approximation (see the section between equation (4.2.24) and (4.2.25)) where the full evolution is replaced by no evolution rather than by free evolution although one is in the Schrödinger picture. Correcting this point one obtains instead the result (21) with the Cluster expansion approach.

### 4.3. Green’s function approach

In the Green’s function approach one starts with general dynamic equations for the two-time correlator  $G^<(t_1, t_2)$ . However, solving such equations is generally difficult and therefore some approximation that limits the equations to the time-diagonal  $t_2 = t_1$  is desirable. This is also necessary if one wants to derive a Boltzmann type equation for  $\rho(t_1) = G^<(t_1, t_1)$ . We start with the discussion of the Ansatz and then turn to the derivation of semiclassical kinetic equations from the Kadanoff–Baym equations. However, we will see that even for a given Ansatz one can derive different collision integrals.

*4.3.1. The problem of the Ansatz.* The first proposed Ansatz was the Kadanoff–Baym (KB) Ansatz [37]

$$G^<(x, p, t, \omega) = \rho(x, p, t)A(x, p, t, \omega) \quad (36)$$

with  $A = i(G^R - G^A)$  being the nonequilibrium spectral function. This is a slight nonequilibrium modification of the equilibrium result  $G^<(k, \omega) = f_{\text{FD}}(\omega)A(k, \omega)$  (the fluctuation-dissipation theorem) and therefore it is expected to be a good approximation close to equilibrium. For weak interactions one uses the quasiparticle approximation  $A \approx 2\pi(\epsilon_k - \omega)$ .

For nonequilibrium beyond a linear response the KB Ansatz fails. This was noted by Jauho and Wilkins [51]–[53] in Boltzmann treatments of transport in strong electric fields, where their results differed from those [54] derived with density matrix methods. A similar discrepancy was observed in the linear conductivity when comparing with Kubo formula calculations [55]. Later Lipavsky *et al* showed that the discrepancy could be cured with the modified Ansatz and coined the generalized Kadanoff–Baym Ansatz (GKBA) [38] (see also [30, 39])

$$\begin{aligned} G^<(\mathbf{x}_1, t_1, \mathbf{x}_2, t_2) &= i \int d^2x_3 (G^R(\mathbf{x}_1, t_1, \mathbf{x}_3, t_2)G^<(\mathbf{x}_1, t_2, \mathbf{x}_2, t_2) \\ &\quad - G^<(\mathbf{x}_1, t_1, \mathbf{x}_2, t_1)G^A(\mathbf{x}_3, t_1, \mathbf{x}_2, t_2)) \\ &= iG^R(t_1, t_2)\rho(t_2) - i\rho(t_1)G^A(t_1, t_2) \end{aligned} \quad (37)$$

(spatial variables suppressed in the latter expression) which reduces to the KB Ansatz in equilibrium. Reference [38] showed that the right-hand side is the first term in an exact expansion, which makes it possible to address the range of validity of the Ansatz. The exact expression respects the causal structure of the Kadanoff–Baym or Keldysh equations and also fulfils some other natural criteria (see appendix B). Semiclassical gradient expansion and electric field modifications can now be treated in a more consistent way.

The GKB Ansatz seems to be most common alternative in applications when the KB Ansatz is considered insufficient. Interestingly, however, in general it does not give the same Boltzmann equation as the one derived with the earlier mentioned density matrix approaches (Liouville equation approaches). For the first quantum correction of graphene the difference matters.

However, we do find an Ansatz for which the kinetic equation obtained with a density matrix approach is also obtained from a Green’s function approach, namely if the GKBA is replaced by the anti-ordered version (AA for anti-ordered Ansatz)

$$G^<(t_1, t_2) = iG^<(t_1, t_1)G^R(t_1, t_2) - iG^A(t_1, t_2)G^<(t_2, t_2) \\ = i\rho(t_1)G^R(t_1, t_2) - iG^A(t_1, t_2)\rho(t_2). \quad (38)$$

Although this Ansatz violates the causal retarded-lesser-advanced structure of KB equations and the Langreth–Wilkins rules [56], it can be derived in a similar way to the GKBA (see appendix B). The full result (including the omitted expansion terms) fulfils almost all the criteria required in [38], in particular the causality requirement. The average of GKBA and the AA gives a third alternative, here named the symmetrized Kadanoff–Baym Ansatz (SKBA),

$$G^<(t_1, t_2) = \frac{1}{2} (\rho(t_1)A(t_1, t_2) + A(t_1, t_2)\rho(t_2)). \quad (39)$$

This Ansatz to zeroth order in the gradient expansion appears for example in [25].

Considering the importance that the issue of Ansatz carries for spinless electrons in nonequilibrium beyond the linear response, we believe that the issue should be even more important for graphene calculations beyond the linear response, at least when electron–hole coherent effects have to be taken into account.

*4.3.2. The problem of identifying the collision integral.* The generalized Kadanoff–Baym equation [37, 56] reads

$$G^< = G^R \Sigma^< G^A + (1 + G^R \Sigma^R) G^{0<} (1 + \Sigma^A G^A) \quad (40)$$

where all products are to be interpreted as convolution products in real space/time and in spin variables. The retarded and advance components are determined by the Dyson equations  $((G^0)^{-1} - \Sigma^R)G^R = 1$  and  $((G^0)^{-1} - \Sigma^A)G^A = 1$ . The self-energies are to first order Born approximation given by

$$\Sigma^< = n_{\text{imp}} V G^< V, \quad \Sigma^{R,A} = n_{\text{imp}} (V + V G^{0R,A} V) \rightarrow n_{\text{imp}} V G^{0R,A} V, \quad (41)$$

where we will neglect the mean-field terms  $\sim V^1$  as we are not interested in shifts of the total energy in this paper.

The term containing  $G^{0<}$  in (40) plays the role of boundary conditions and vanishes when acting with  $(G^R)^{-1}$  from the left or  $(G^A)^{-1}$  from the right,

$$(G^R)^{-1}G^< = \Sigma^<G^A, \quad G^<(G^A)^{-1} = G^R\Sigma^<. \quad (42)$$

In particular, the difference gives the Kadanoff–Baym equation in differential form, which is a double-time precursor of the time-diagonal kinetic equations to be derived. For our discussion we want to write it in two ways. The first equation, to be called G1, is

$$[i\partial_t - H, G^<] = \Sigma^R G^< - G^< \Sigma^A + \Sigma^< G^A - G^R \Sigma^<. \quad (43)$$

It identifies all the self-energy terms of order  $V^2$  with the collision integral. This is what we think should be done for a comparison with the Liouville equation based approaches of the previous sections, where all terms of order  $V^2$  were identified with the collision integral. The second equation, to be called G2, is given by

$$[i\partial_t - H - \text{Re} \Sigma^R, G^<] - [\Sigma^<, \text{Re} G^R] = i\{\text{Im} \Sigma^R, G^<\} - i\{\Sigma^<, \text{Im} G^R\}. \quad (44)$$

It is a frequently encountered starting point of Boltzmann treatments that consider renormalizations and other quantum corrections [30, 39, 56, 57]. Of the self-energy terms, only those on the right-hand side are considered as the collision integral, those on the left-hand side, in contrast, as terms renormalizing the free drift. (The term  $\text{Re} \Sigma^R$ , for example, shifts the zero of energy. Thereby it horizontally shifts the conductivity as a function of gate voltage, e.g. shifts the minimum conductivity away from zero gate voltage. In this context, see experiments [12, 13].) For spinless electrons the commutators on the left-hand side vanish if one stops at zeroth order in the gradient expansion. In this case one obtains the same collision integral to zeroth order in the gradient expansion as with (43). In general, however, and in particular the case of spin, the self-energy terms on the left-hand side contribute even to zeroth order. We hope to address such renormalization corrections in future work. In the present paper we are mainly interested in the alternative structures that might be obtained for a collision integral from the right-hand side in (44).

Both equations (43) and (44) also hold for  $G^>$ . Within the Keldysh formalism the same equations are derived for  $G^K = i(G^< - G^>)$ .

Notice that the *quantum Boltzmann equation* [57], obtained by gradient expanding (44) to first order, is a semiclassical kinetic equation in the variables  $(\mathbf{x}, \mathbf{p}, t, \omega)$ . Integrating the resulting equation over the frequency (independent energy)  $\omega$  gives a Boltzmann equation<sup>13</sup>. In this sense we solve Boltzmann equations in this paper, not quantum Boltzmann equations.

**4.3.3. Different collision integrals.** With two different ways of writing the Kadanoff–Baym equation and three different kinds of Ansatz there are possibly six new collision integrals. One obvious question is, which of them corresponds to the collision integrals of section 4.3.2. The second and *independent* question is, which one is appropriate for the problem of quantum corrections to the conductivity in graphene.

<sup>13</sup> One can also integrate over the absolute value of the momentum to get a Boltzmann equation in terms of the variables  $(\mathbf{x}, \hat{\mathbf{p}}, t, \omega)$ . This is called the quasiclassical approach and is used for example in [24, 25]. (Sometimes it is called the *first* quasiclassical approach and the semiclassical approach is instead called the quasiclassical approach [30].)

In this paper we believe we are able to present an answer to the first question. It seems clear that the pertinent collision integral is derived from G1, that is (43). The question is what Ansatz to choose. Interestingly, it is not the GKB Ansatz, but the AA that returns the collision integral (21). The GKBA would give

$$\begin{aligned} \Sigma^R G^< - G^< \Sigma^A + \Sigma^< G^A - G^R \Sigma^< \\ &= -iV G^{0R} V \rho G^{0A} - iG^{0R} \rho V G^{0A} V + iV G^{0R} \rho V G^{0A} + iG^{0R} V \rho G^{0A} V + \dots \\ &= -i[V, G^{0R}[V, \rho]G^{0A}] + \dots \end{aligned} \quad (45)$$

where, in each term like  $\Sigma^R G^< = V G^{0R} V G^{0R} \rho - V G^{0R} V \rho G^{0A}$ , we neglected the parts that contain two retarded or two advanced Green's functions since such terms vanish when one integrates over the frequency to obtain the collision integral,

$$\mathcal{J} = - \int \frac{d\omega}{2\pi} [V, G^{0R}[V, \rho]G^{0A}]. \quad (46)$$

We call this collision integral G1wGKBA (w for with). It is clearly different from (21). Interestingly it coincides with (26).

For the collision integrals G2 derived from (44) note, for example, that with the GKBA we obtain

$$\frac{1}{2}\{\Sigma^R - \Sigma^A, G^<\} - \frac{1}{2}\{\Sigma^<, G^R - G^A\} = -\frac{1}{2}[V, G^{0R}[V, \rho]G^{0A}] - \frac{1}{2}[V, [G^{0A} V G^{0R}, \rho]]. \quad (47)$$

We denote this collision integral G2wGKBA. It takes the form of an average of (46) and (21), in the latter, however, with retarded and advanced Green's functions swapped. The other possible collision integrals are presented in section 5.

## 5. Comparing collision integrals for graphene

The different possible general collision integrals discussed in section 4 will now be summarized. When writing  $\mathcal{J}[\rho] = - \int (d\omega/2\pi)(\dots)$  the integrands  $(\dots)$  of the various candidates are given by

vN&	G1	GKBA	[V, G <sup>0R</sup> [V, ρ]G <sup>0A</sup> ]	
	G1	AA	[V, [G <sup>0R</sup> V G <sup>0A</sup> , ρ]]	
	G1	SKBA	$\frac{1}{2}[V, G^{0R}[V, \rho]G^{0A}] + \frac{1}{2}[V, [G^{0R}V G^{0A}, \rho]]$	
	G2	GKBA	$\frac{1}{2}[V, G^{0R}[V, \rho]G^{0A}] + \frac{1}{2}[V, [G^{0A}V G^{0R}, \rho]]$	(48)
	G2	AA	$\frac{1}{2}[V, G^{0A}[V, \rho]G^{0R}] + \frac{1}{2}[V, [G^{0R}V G^{0A}, \rho]]$	
	G2	SKBA	$\frac{1}{2}(G2wGKBA + G2wAA)$	
NSO			[G <sup>0R</sup> V G <sup>0A</sup> , [V, ρ]].	

We do not have to solve the Boltzmann equation seven times since the first two cases are sufficient to deduce all cases except the NSO case, which, however, will turn out to coincide with the G1wAA/vN calculation. For example, the second term of G2wGKBA is similar to the G1wAA result with retarded and advanced Green's functions swapped. A closer inspection (see appendix A) reveals that this swapping has no effect on the delta function part of the collision integral, but changes the sign of the principal value part. Therefore the delta function part of G2wGKBA is given by the delta function part of (G1wGKBA + G1wAA)/2, whereas the principal value part is given by the principal

value part of  $(G1wGKBA - G1wAA)/2$ . One can decompose the principal value part of G1wGKBA into two parts  $X$  and  $Y$ , where  $X$  is the part that is invariant when one compares G1wAA with G1wGKBA, whereas  $Y$  is the part that changes sign. Then one can work out the principal value parts  $\mathcal{J}^P = \pm \mathcal{J}^{PX} \pm \mathcal{J}^{PY}$  for all the above collision integrals, with the relative signs of  $\mathcal{J}^{PX}$  and  $\mathcal{J}^{PY}$ , respectively, determined by the scheme

		$X$	$Y$
G1	GKBA	+	+
G1	AA	+	-
G1	SKBA	+	0
G2	GKBA	0	+
G2	AA	0	-
G2	SKBA	0	0.

(49)

Note in particular that for the collision integral G2wSKBA the principal value terms vanish completely.

The products in (48) are still general convolutions. At this point the spin structure is left intact but the space and time variables are Wigner transformed and the products are then gradient expanded in these variables. We now assume that gradient corrections in the interaction terms can be neglected. We also replace the Wigner transformed density matrix  $\rho$  with the quasiparticle distribution  $f$ . These are two approximations which might be incorrect when calculating quantum corrections, but give the framework within which we want to make a first step and compare with previous work. Furthermore, we assume non-magnetic impurities,  $u_{\mathbf{k}\mathbf{k}'}^{\sigma\sigma'} = \delta_{\sigma\sigma'} u_{\mathbf{k}\mathbf{k}'}$  with  $W_{\mathbf{k}\mathbf{k}'} := 2\pi n_{\text{imp}} |u_{\mathbf{k}\mathbf{k}'}|^2$ . After impurity averaging the collision integrals become

$$\begin{aligned}
 \text{G1wGKBA} \quad \mathcal{J}[f(\mathbf{k}, \mathbf{x}, t)] &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \int \frac{d\omega}{(2\pi)^2} (G_{\mathbf{k}}^{0R} \Delta f G_{\mathbf{k}'}^{0A} + G_{\mathbf{k}'}^{0R} \Delta f G_{\mathbf{k}}^{0A}), \\
 \text{vN} \quad \mathcal{J}[f(\mathbf{k}, \mathbf{x}, t)] &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \int \frac{d\omega}{(2\pi)^2} (f_{\mathbf{k}} G_{\mathbf{k}}^{0R} G_{\mathbf{k}'}^{0A} - f_{\mathbf{k}'} G_{\mathbf{k}'}^{0R} G_{\mathbf{k}}^{0A} + \text{h.c.}), \\
 \text{NSO} \quad \mathcal{J}[f(\mathbf{k}, \mathbf{x}, t)] &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \int \frac{d\omega}{(2\pi)^2} (\Delta f G_{\mathbf{k}'}^{0R} G_{\mathbf{k}}^{0A} + G_{\mathbf{k}}^{0R} G_{\mathbf{k}'}^{0A} \Delta f),
 \end{aligned} \tag{50}$$

to second order in the interaction and to zeroth order in the gradient expansion. The shorthand notations  $\int d^2k'/(2\pi)^2 =: \int_{\mathbf{k}'}$  and  $\Delta f = f(\mathbf{k}, \mathbf{x}, t) - f(\mathbf{k}', \mathbf{x}, t)$  were introduced. The retarded Green's function is the non-interacting one taken to lowest order in the gradient expansion. For the spin-orbit coupled case it is of the form

$$G_{\mathbf{k}}^{0R} = \sum_{s=\pm} \frac{S_{\hat{\mathbf{b}}_s}}{\tilde{\omega}^+ - \epsilon_{\mathbf{k}}^s}, \quad S_{\hat{\mathbf{b}}_s} := \frac{1}{2}(\mathbf{1} + \boldsymbol{\sigma} \cdot s\hat{\mathbf{b}}_{\mathbf{k}}) \tag{51}$$

with  $\tilde{\omega}^+ = \tilde{\omega} + i0^+$  and with  $\tilde{\omega} = \omega - \phi$  being the gauge invariant frequency variable. In the Wigner representation one has  $X^A = (X^R)^\dagger$ .

The three collision integrals in (50) would obviously be equivalent if the ingredients  $G^{0R}$ ,  $G^{0A}$  and  $f$  commuted with each other, as is the case for spinless electrons. In the general non-commuting case, including the case of spin-orbit coupling, the collision integrals appear to be different. However, the different forms do not necessarily imply differing results. We will find that to lowest order in  $(\ell k_F)^{-1}$  they all reproduce the Drude

conductivity obtained with Fermi's Golden rule. To higher order in quantum corrections, however, an agreement is not at all obvious.

Notice that the collision integral for non-magnetic impurities should generally satisfy the property  $\int_{\mathbf{k}} \mathcal{J}[f(\mathbf{k}, \mathbf{x}, t)] = 0$ , expressing that in real space  $(\mathbf{x}, t)$  the collisions cannot act as a source or drain of particles of a given spin state. For all collision integrals except the NSO integral this is manifest since the collision integrals change sign under the renaming of dummy variables  $\mathbf{k} \leftrightarrow \mathbf{k}'$ . In the case of the NSO result this is not manifest at this level, but the explicit collision integral derived for graphene will turn out to have this property.

For further comparison and for the explicit solution of the Boltzmann equation we will write the collision integrals (50) explicitly in terms of the components  $f_0$  and  $\mathbf{f}$ . To streamline the lengthy expressions some more shorthand notation is introduced.  $x'$  means that the quantity  $x$  depends on primed variables such as  $\mathbf{k}'$ ,  $s'$  etc, whereas  $x$  correspondingly depends on  $\mathbf{k}$ ,  $s$ . For example  $S' = \frac{1}{2}(\mathbf{1} + \boldsymbol{\sigma} \cdot s' \hat{\mathbf{b}}_{\mathbf{k}'})$ . Also,  $\Delta x := x - x'$ , for example  $\Delta \epsilon = \epsilon_{\mathbf{k}}^s - \epsilon_{\mathbf{k}'}^{s'}$  and  $\Delta(sb) = sb - s'b'$ .

Inserting (51) into (50) gives a collision integral  $\mathcal{J} = \mathcal{J}^\delta + \mathcal{J}^P$  consisting of delta function terms and of principal value terms. The principal value part terms  $\mathcal{J}^P$  are given by

$$\begin{aligned}
 \text{G1wGKBA} \quad \mathcal{J}^P[f] &= \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \frac{1}{2\pi} \sum_{ss'} \mathcal{P} \left( \frac{1}{\Delta \epsilon} \right) \\
 &\times \left[ \frac{ss' \hat{\mathbf{b}} \times \hat{\mathbf{b}}'}{2} \cdot (-\Delta \mathbf{f} + \boldsymbol{\sigma} \Delta f_0) + \boldsymbol{\sigma} \cdot \frac{\Delta(sb)}{2} \times \Delta \mathbf{f} \right], \\
 \text{vN \& NSO} \quad \mathcal{J}^P[f] &= \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \frac{1}{2\pi} \sum_{ss'} \mathcal{P} \left( \frac{1}{\Delta \epsilon} \right) \\
 &\times \left[ \frac{ss' \hat{\mathbf{b}} \times \hat{\mathbf{b}}'}{2} \cdot (+\Delta \mathbf{f} + \boldsymbol{\sigma} \Delta f_0) + \boldsymbol{\sigma} \cdot \frac{s\hat{\mathbf{b}} + s'\hat{\mathbf{b}}'}{2} \times \Delta \mathbf{f} \right].
 \end{aligned} \tag{52}$$

The delta function terms are given by

$$\begin{aligned}
 \mathcal{J}_0^\delta[f] &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \frac{1}{2} \sum_{ss'} \delta(\Delta \epsilon) \left[ \frac{1 + ss' \hat{\mathbf{b}} \cdot \hat{\mathbf{b}}'}{2} \Delta f_0 + \frac{s\hat{\mathbf{b}} + s'\hat{\mathbf{b}}'}{2} \cdot \Delta \mathbf{f} \right], \\
 \mathcal{J}^\delta[f] &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \frac{1}{2} \sum_{ss'} \delta(\Delta \epsilon) \left[ \Delta \left( \frac{1 + ss' B}{2} \mathbf{f} \right) + \frac{s\hat{\mathbf{b}} + s'\hat{\mathbf{b}}'}{2} \Delta f_0 \right],
 \end{aligned} \tag{53}$$

with the matrix  $B(\hat{\mathbf{k}}, \hat{\mathbf{k}}')$  acting on  $\mathbf{f}$  given by

$$\begin{aligned}
 \text{G1wGKBA} \quad B &:= +\hat{\mathbf{b}}(\hat{\mathbf{b}}')^T + \hat{\mathbf{b}}'(\hat{\mathbf{b}})^T - \hat{\mathbf{b}} \cdot \hat{\mathbf{b}}', & B' &:= B \\
 \text{vN} \quad B &:= -\hat{\mathbf{b}}(\hat{\mathbf{b}}')^T + \hat{\mathbf{b}}'(\hat{\mathbf{b}})^T + \hat{\mathbf{b}} \cdot \hat{\mathbf{b}}', & B' &:= B^T \\
 \text{NSO} \quad B &:= +\hat{\mathbf{b}}(\hat{\mathbf{b}}')^T - \hat{\mathbf{b}}'(\hat{\mathbf{b}})^T + \hat{\mathbf{b}} \cdot \hat{\mathbf{b}}', & B' &:= B \\
 \text{rest} \quad B &:= \hat{\mathbf{b}}'(\hat{\mathbf{b}})^T, & B' &:= B^T.
 \end{aligned} \tag{54}$$

The 'rest' stands for the G1wSKBA as well as all G2 collision integrals. As stated above, their delta function parts are just the sum of G1wGKBA and G1wAA/vN. Taking into

account the momentum dependence of the basis vectors

$$\hat{\mathbf{b}}' = \hat{\mathbf{b}} \cos N\Delta\theta - \hat{\mathbf{c}} \sin N\Delta\theta, \quad \hat{\mathbf{c}}' = \hat{\mathbf{c}} \cos N\Delta\theta + \hat{\mathbf{b}} \sin N\Delta\theta, \quad (55)$$

one derives

G1wGKBA	vN	NSO	rest	
$B\hat{\mathbf{b}} = \hat{\mathbf{b}}'$	$B\hat{\mathbf{b}} = \hat{\mathbf{b}}'$	$B\hat{\mathbf{b}} = \hat{\mathbf{b}} \cos N\Delta\theta + \hat{\mathbf{c}} \sin N\Delta\theta$	$B\hat{\mathbf{b}} = \hat{\mathbf{b}}'$	(56)
$B'\hat{\mathbf{b}}' = \hat{\mathbf{b}}$	$B'\hat{\mathbf{b}}' = \hat{\mathbf{b}}$	$B'\hat{\mathbf{b}}' = \hat{\mathbf{b}}$	$B'\hat{\mathbf{b}}' = \hat{\mathbf{b}}$	
$B\hat{\mathbf{c}} = -\hat{\mathbf{c}}'$	$B\hat{\mathbf{c}} = \hat{\mathbf{c}}'$	$B\hat{\mathbf{c}} = \hat{\mathbf{c}} \cos N\Delta\theta - \hat{\mathbf{b}} \sin N\Delta\theta$	$B\hat{\mathbf{c}} = 0$	
$B'\hat{\mathbf{c}}' = -\hat{\mathbf{c}}$	$B'\hat{\mathbf{c}}' = \hat{\mathbf{c}}$	$B'\hat{\mathbf{c}}' = -\hat{\mathbf{c}}$	$B'\hat{\mathbf{c}}' = 0$	

Note the particular simplicity of the approaches G1wSKBA and G2.

For studies where a spin-coherent Boltzmann equation is linearized in a small  $b$  ( $b_F \ll \epsilon_F$ ) the terms  $ss'B$  do not appear. Also, it should be safe to neglect the principal value terms if one is only interested in the response without quantum corrections. In that case, the delta function part of the collision integral is the same in all formalisms [27]. However, for graphene ( $\epsilon_F = b_F$ ) we need the full collision integral to calculate the quantum corrections and the approaches therefore differ. However, a crucial simplification comes through  $\epsilon^\pm = \pm b$  due to  $\epsilon_0 = 0$ . With  $\Delta\epsilon = sb - s'b'$  we obtain (henceforth we write  $\mathcal{P}(1/x)$  as  $1/x$ )

$$\begin{aligned} \sum_{ss'} \delta(\Delta\epsilon) &= 2(\delta(\Delta b) + \delta(b + b')) & \sum_{ss'} s\delta(\Delta\epsilon) &= \sum_{ss'} s'\delta(\Delta\epsilon) = 0 \\ \sum_{ss'} ss'\delta(\Delta\epsilon) &= 2(\delta(\Delta b) - \delta(b + b')) & \sum_{ss'} \frac{1}{\Delta\epsilon} &= \sum_{ss'} ss' \frac{1}{\Delta\epsilon} = 0 \\ \sum_{ss'} s \frac{1}{\Delta\epsilon} &= 2 \left( \frac{1}{\Delta b} + \frac{1}{b + b'} \right) & \sum_{ss'} s' \frac{1}{\Delta\epsilon} &= 2 \left( \frac{1}{\Delta b} - \frac{1}{b + b'} \right) \end{aligned} \quad (57)$$

and therefore half of the terms in (53) vanish, leaving

$$\begin{aligned} \mathcal{J} = - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} & \left\{ \delta(\Delta b) \left( \cos^2 \frac{\Delta\theta}{2} \Delta f_0 + \boldsymbol{\sigma} \cdot \Delta \left( \frac{1+B}{2} \mathbf{f} \right) \right) \right. \\ & + \delta(b + b') \left( \sin^2 \frac{\Delta\theta}{2} \Delta f_0 + \boldsymbol{\sigma} \cdot \Delta \left( \frac{1-B}{2} \mathbf{f} \right) \right) \\ & \left. + \frac{1}{\pi\Delta b} \boldsymbol{\sigma} \cdot (\hat{\mathbf{b}} + \kappa\hat{\mathbf{b}}') \times \Delta \mathbf{f} + \frac{1}{\pi(b + b')} \boldsymbol{\sigma} \cdot (\hat{\mathbf{b}} - \kappa\hat{\mathbf{b}}') \times \Delta \mathbf{f} \right\}. \end{aligned} \quad (58)$$

Notice that the equations for the charge  $f_0$  and the spin  $\mathbf{f}$  are completely decoupled for graphene.

To obtain the principal value terms for G1wGKBA, let  $\kappa = -$  and for G1wAA/vN/NSO let  $\kappa = +$ . The principal value terms of the other cases can be constructed out of these. The term with  $\delta(b + b')$  gives only a contribution from the point  $k = -k'$ , i.e.  $k = k' = 0$  which we will neglect<sup>14</sup> since we consider  $k_F \neq 0$ . (This term assures formally a continuity in the conductivity when  $k_F = 0^+ \rightarrow k_F = 0$ .) Thus,

<sup>14</sup> Auslender communicated to us that in a careful NSO treatment this term can be canceled by an equivalent term coming from the  $\mathcal{J}^{(1)}$  part in  $\mathcal{J}^{(2)}$ .

the delta function part we consider is

$$\mathcal{J}^\delta[\mathbf{f}] = - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \delta(\Delta b) \frac{1}{2} (\mathbf{f} - \mathbf{f}' + B\mathbf{f} - B'\mathbf{f}'). \quad (59)$$

For the approach G1wGKBA and for all G2 approaches we obtain due to (56)

$$\mathcal{J}^\delta[\mathbf{f}] = - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \delta(\Delta b) \Delta \left( \frac{1+B}{2} \hat{\mathbf{b}} f_{\hat{\mathbf{b}}} \right) - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \delta(\Delta b) \frac{1}{2} \Delta (\hat{\mathbf{c}} f_{\hat{\mathbf{c}}} + \hat{\mathbf{z}} f_z) \quad (60)$$

for the components  $\mathbf{f} = \hat{\mathbf{b}} f_{\hat{\mathbf{b}}} + \hat{\mathbf{c}} f_{\hat{\mathbf{c}}} + \hat{\mathbf{z}} f_z$ . In section 6 we will see that the matrix  $(1+B)/2$  is responsible for the additional chirality-induced spin-overlap factor  $\cos^2(N\Delta\theta/2)$  occurring in the intra-band transition rates involving only the probability densities  $\langle \hat{\mathbf{b}} \pm | f | \hat{\mathbf{b}} \pm \rangle = f_0 \pm f_{\hat{\mathbf{b}}}$  of energy eigenstates. This is how the Drude conductivity found with Fermi's Golden rule builds in the suppression of backscattering in monolayer graphene ( $N = \pm 1$ ). The 'transition amplitudes' involving the off-diagonal components  $\langle \hat{\mathbf{b}} \pm | f | \hat{\mathbf{b}} \mp \rangle = f_z \pm i f_{\hat{\mathbf{c}}}$  (the Zitterbewegung components) are more elusive and beyond the reach of Fermi's Golden rule. However, for the G1wGKBA and all G2 approaches, the result (60) shows that the scattering of the off-diagonal components becomes very simple since it contains no angle dependent chirality factors but only a factor  $\frac{1}{2}$  compared to ordinary spin independent scattering.

## 6. Conductivity of graphene with principal value terms neglected

In this section we calculate the electrical conductivity of graphene for non-magnetic impurities with the collision integrals  $\mathcal{J}^\delta$  given in section 5. We neglect the principal value part  $\mathcal{J}^P$ . We also assume low temperature so that  $|\mu| = \epsilon_F$ . For notational compactness we henceforth neglect the charge unit  $e$ , allowing it to appear only in final results.

Before we start, for comparison purposes, we will derive the Drude conductivity per valley by considering only one band (electrons  $\mu > 0$  or holes  $\mu < 0$ ), in which case we can apply Fermi's Golden rule. Let us consider electrons. For monolayer graphene the one-band Boltzmann equation linearized in the electric field ( $f = f^{\text{eq}} + f^{(E)}$  with  $f^{\text{eq}} = f_{\text{FD}}(v_F k - \mu)$  for electrons) reads

$$\begin{aligned} \mathbf{E} \cdot \partial_{\mathbf{k}} f^{\text{eq}} &= - \int_{\mathbf{k}'} \delta(v_F \Delta k) W_{\mathbf{k}\mathbf{k}'} \cos^2 \frac{\Delta\theta}{2} \Delta f^{(E)} \\ &= - f^{(E)} \underbrace{\int_{\mathbf{k}'} \delta(v_F \Delta k) W_{\mathbf{k}\mathbf{k}'} \cos^2 \frac{\Delta\theta}{2} (1 - \cos \Delta\theta)}_{=: \tau_{\text{tr}}^{-1}}, \end{aligned} \quad (61)$$

where the transition probability  $W_{\mathbf{k}\mathbf{k}'} \cos^2 \Delta\theta/2$  (contrast with  $W_{\mathbf{k}\mathbf{k}'}$  for ordinary electrons) takes into account the chirality of the Dirac electrons, responsible for the suppression of backscattering. The real space current is given by

$$\mathbf{j} = \int_{\mathbf{k}'} \mathbf{v} f^{(E)} = - \int_{\theta'} \int \frac{k \, dk}{2\pi} v_F \hat{\mathbf{k}} \tau_{\text{tr}} E_{\hat{\mathbf{k}}} \partial_{\mathbf{k}} f_{\text{FD}}(v_F k - \mu) = \mathbf{E} \sigma_0 \quad (62)$$

where (reintroducing  $e$  and  $\hbar$  to the right)

$$\sigma_0 := \frac{|\mu| \tau_{\text{trF}}}{4\pi} = \frac{\ell k_F}{4\pi} \rightarrow \frac{e^2}{2\hbar} \ell k_F \quad (63)$$

with  $\tau_{\text{trF}} := \tau_{\text{tr}}(k_{\text{F}})$ ,  $k_{\text{F}} \equiv |\mu|/v_{\text{F}}$  and the mean free path  $\ell := v_{\text{F}}\tau_{\text{trF}}$ . In (62) we used the shorthand notation  $\int_{\theta} := 1/2\pi \int d\theta$ . The result (63) is written in such a way that it also includes the case of holes ( $\mu < 0$ ). To get the total Drude conductivity of graphene we multiply by a factor of four for the degeneracy in valley index and real spin.

We turn to the coherent treatment of pseudospin and see that all approaches reproduce (63) to lowest order in  $(\ell k_{\text{F}})^{-1}$  but give different quantum corrections. With

$$K(k, \theta, \theta') := \int_0^{\infty} \frac{k' dk'}{2\pi} W_{\mathbf{k}\mathbf{k}'} \delta(b - b'), \quad (64)$$

the compact notation  $\mathbf{E} \cdot \partial_{\mathbf{k}} = E_{\hat{\mathbf{k}}} \partial_{\mathbf{k}} + E_{\hat{\theta}}(1/k) \partial_{\theta}$ , the decomposition  $f = f_0 + \boldsymbol{\sigma} \cdot (\hat{\mathbf{b}} f_{\hat{\mathbf{b}}} + \hat{\mathbf{c}} f_{\hat{\mathbf{c}}} + \hat{\mathbf{z}} f_z)$  with  $\partial_{\theta} \hat{\mathbf{b}} = N \hat{\mathbf{c}}$  and  $\partial_{\theta} \hat{\mathbf{c}} = -N \hat{\mathbf{b}}$  and using the table (56) we find for G1wGKBA

$$\begin{aligned} \mathbf{E} \cdot \partial_{\mathbf{k}} f_0 &= \mathcal{J}_0^{\delta} = - \int_{\theta'} K \cos^2 \frac{N\Delta\theta}{2} \Delta f_0, \\ \mathbf{E} \cdot \partial_{\mathbf{k}} f_{\hat{\mathbf{b}}} - E_{\hat{\theta}} \frac{N}{k} f_{\hat{\mathbf{c}}} &= \mathcal{J}_{\hat{\mathbf{b}}}^{\delta} = - \int_{\theta'} K \left( \cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{b}}} - \frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{c}}} + f_{\hat{\mathbf{c}}}') \right), \\ \mathbf{E} \cdot \partial_{\mathbf{k}} f_{\hat{\mathbf{c}}} + E_{\hat{\theta}} \frac{N}{k} f_{\hat{\mathbf{b}}} + 2b f_z &= \mathcal{J}_{\hat{\mathbf{c}}}^{\delta} = - \int_{\theta'} K \left( \sin^2 \frac{N\Delta\theta}{2} (f_{\hat{\mathbf{c}}} + f_{\hat{\mathbf{c}}}') - \frac{1}{2} \sin N\Delta\theta \Delta f_{\hat{\mathbf{b}}} \right), \\ \mathbf{E} \cdot \partial_{\mathbf{k}} f_z - 2b f_{\hat{\mathbf{c}}} &= \mathcal{J}_z^{\delta} = - \int_{\theta'} K \sin^2 \frac{N\Delta\theta}{2} \Delta f_z. \end{aligned} \quad (65)$$

The other collision integrals are obtained with the ingredients in  $\mathcal{J}_{\mu}^{\delta}$  replaced according to the following table

	$\mathcal{J}_0^{\delta}$	$\mathcal{J}_{\hat{\mathbf{b}}}^{\delta}$	$\mathcal{J}_{\hat{\mathbf{c}}}^{\delta}$	$\mathcal{J}_z^{\delta}$
G1wG.	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_0$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{b}}}$ $-\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{c}}}' + f_{\hat{\mathbf{c}}})$	$\sin^2 \frac{N\Delta\theta}{2} (f_{\hat{\mathbf{c}}} + f_{\hat{\mathbf{c}}}' )$ $+\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{b}}}' - f_{\hat{\mathbf{b}}})$	$\sin^2 \frac{N\Delta\theta}{2} \Delta f_z$
vN	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_0$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{b}}}$ $-\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{c}}}' - f_{\hat{\mathbf{c}}})$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{c}}}$ $+\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{b}}}' - f_{\hat{\mathbf{b}}})$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_z$
NSO	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_0$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{b}}}$ $-\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{c}}}' + f_{\hat{\mathbf{c}}})$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{c}}}$ $+\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{b}}}' + f_{\hat{\mathbf{b}}})$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_z$
rest	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_0$	$\cos^2 \frac{N\Delta\theta}{2} \Delta f_{\hat{\mathbf{b}}}$ $-\frac{1}{2} \sin N\Delta\theta f_{\hat{\mathbf{c}}}'$	$\frac{1}{2} f_{\hat{\mathbf{c}}} - \frac{1}{2} \cos N\Delta\theta f_{\hat{\mathbf{c}}}'$ $+\frac{1}{2} \sin N\Delta\theta (f_{\hat{\mathbf{b}}}' - f_{\hat{\mathbf{b}}})$	$\frac{1}{2} \Delta f_z$ .

(66)

All terms including the trigonometric factor  $\sin \Delta N\theta$  are, in the assumed case of symmetric scattering  $K(\Delta\theta) = K(-\Delta\theta)$ , actually the same in all approaches since only the part including  $f'$  can survive, whereas the part including  $f$  vanishes trivially. Thus, the approaches differ only in the elements  $\mathcal{J}_{\hat{\mathbf{c}}}[f_{\hat{\mathbf{c}}}]$  and  $\mathcal{J}_z[f_z]$ . These, however, will only enter the solution to order  $\sim(\ell k_{\text{F}})^{-1}$ . We will see that the first quantum correction to the conductivity will depend on  $\mathcal{J}_z[f_z]$ . Since the iterative solution in Culcer *et al* [22] was only taken to order  $(\ell k_{\text{F}})^0$  the choice of Markov approximation, and in general the choice of formalism, would not have mattered.

For further comparison with [22], notice that equation (12b) for  $P_{\perp} \mathcal{J}[S_{\parallel}]$  (our  $\mathcal{J}_{\hat{\mathbf{c}}}[f_{\hat{\mathbf{b}}}]$ ) and equation (12c) for  $P_{\parallel} \mathcal{J}[S_{\perp}]$  (our  $\mathcal{J}_{\hat{\mathbf{b}}}[f_{\hat{\mathbf{c}}}]$ ) exactly match the G1wGKBA collision

integral above. The comparison was, however, already established at an earlier stage (26). At the present stage, on the contrary, a comparison with the NSO derived collision integral of Auslender *et al* [20] is also possible, see appendix C.

We proceed by linearizing the equations in the electric field with  $f = f^{\text{eq}} + f^{(E)}$  and by Fourier decomposing the components of  $f_r^{(E)} = \sum_n e^{in\theta} f_{rn}^{(E)}$ , ( $r = 0, \hat{\mathbf{b}}, \hat{\mathbf{c}}, z$ ). In equilibrium we have

$$f_0^{\text{eq}} \pm f_{\hat{\mathbf{b}}}^{\text{eq}} = f_{\text{FD}}(\pm v_{\text{F}}k) = \Theta(\mu \mp v_{\text{F}}k) + \mathcal{O}((k_{\text{B}}T/\epsilon_{\text{F}})^2), \quad f_{\hat{\mathbf{c}}}^{\text{eq}} = f_z^{\text{eq}} = 0. \quad (67)$$

Since  $\mathbf{E} \cdot \partial_k f^{\text{eq}}$  with

$$\mathbf{E} \cdot \partial_k f_{\text{FD}}(\epsilon^{\pm}) = E_{\hat{\mathbf{k}}} \partial_k f_{\text{FD}}(\epsilon^{\pm}) = \frac{e^{i\theta} \mathcal{E}^* + e^{-i\theta} \mathcal{E}}{2} \partial_k f_{\text{FD}}(\epsilon^{\pm}), \quad E_{\hat{\theta}} = \frac{i}{2}(e^{i\theta} \mathcal{E}^* - e^{-i\theta} \mathcal{E}) \quad (68)$$

(where  $\mathcal{E} := E_x + iE_y$ ) only contains  $n = \pm 1$  Fourier components, we can immediately conclude that  $f_{rn}^{(E)} = 0$  for  $n \neq \pm 1$ . It suffices to study the equation for the  $n = 1$  component because the  $n = -1$  term is just the complex conjugate. We find for the  $n = 1$  Fourier component of the linearized Boltzmann equation

$$\frac{\mathcal{E}^*}{2} \begin{pmatrix} \partial_k f_0^{\text{eq}} \\ \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} \\ i \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} \\ 0 \end{pmatrix} = - \begin{pmatrix} \mathcal{I}^+ & 0 & 0 & 0 \\ 0 & \mathcal{I}^+ & +i\mathcal{I}^s & 0 \\ 0 & -i\mathcal{I}^s & \mathcal{I}^\lambda & 2b \\ 0 & 0 & -2b & \mathcal{I}^\kappa \end{pmatrix} \begin{pmatrix} f_{01}^{(E)} \\ f_{\hat{\mathbf{b}}1}^{(E)} \\ f_{\hat{\mathbf{c}}1}^{(E)} \\ f_{z1}^{(E)} \end{pmatrix}. \quad (69)$$

In terms of the integrals defined below one has  $\mathcal{I}^\kappa = \mathcal{I}^-$  for G1wGKBA and  $\mathcal{I}^\kappa = \mathcal{I}^+$  for G1wAA/vN/NSO. For the G1 wSKBA and all G2 approaches one has  $\mathcal{I}^\kappa = (\mathcal{I}^+ + \mathcal{I}^-)/2$ . Likewise  $\mathcal{I}^\lambda = \tilde{\mathcal{I}}^+$  for G1wGKBA,  $\mathcal{I}^\lambda = \mathcal{I}^+$  for G1wAA/vN/NSO and just the average for the rest,

	for $N = \pm 1$
$\mathcal{I}^+ := \int_{\theta'} K \cos^2 \frac{N\Delta\theta}{2} (1 - e^{-i\Delta\theta}) \equiv \tau_{\text{tr}}^{-1}$	$= \frac{1}{4} \int_{\theta'} K (1 - \cos 2\Delta\theta)$
$\tilde{\mathcal{I}}^+ := \int_{\theta'} K \sin^2 \frac{N\Delta\theta}{2} (1 + e^{-i\Delta\theta})$	$= \mathcal{I}^+$
$\mathcal{I}^- := \int_{\theta'} K \sin^2 \frac{N\Delta\theta}{2} (1 - e^{-i\Delta\theta})$	$= \frac{1}{4} \int_{\theta'} K (3 - 4 \cos \Delta\theta + \cos 2\Delta\theta)$
$i\mathcal{I}^s := - \int_{\theta'} K \frac{\sin N\Delta\theta}{2} e^{-i\Delta\theta} = \frac{i}{2} \int_{\theta'} K \sin N\Delta\theta \sin \Delta\theta$	$\equiv \pm i\mathcal{I}^+$

(70)

where we used that  $K(-\Delta\theta) = K(\Delta\theta)$ . Notice that  $\mathcal{I}^s$  is odd in  $N$  whereas the other integrals  $\mathcal{I}$  are even in  $N$ .

The equation for  $f_0$  is decoupled from the other components and is solved by  $f_{01}^{(E)} = -\frac{1}{2} \mathcal{E}^* \tau_{\text{tr}} \partial_k f_0^{\text{eq}}$  with  $\tau_{\text{tr}} := (\mathcal{I}^+)^{-1}$ . The other components are found by inverting the remaining  $3 \times 3$  matrix,

$$\begin{pmatrix} f_{\hat{\mathbf{b}}1}^{(E)} \\ f_{\hat{\mathbf{c}}1}^{(E)} \\ f_{z1}^{(E)} \end{pmatrix} = -\frac{\mathcal{E}^*}{2|M|} \begin{pmatrix} (4b^2 + \mathcal{I}^\lambda \mathcal{I}^\kappa) \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^s \mathcal{I}^\kappa \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} \\ i\mathcal{I}^\kappa (\mathcal{I}^s \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^+ \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}}) \\ i2b (\mathcal{I}^s \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^+ \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}}) \end{pmatrix}. \quad (71)$$

with the determinant  $|M| = 4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa$ . Adding up the two Fourier components  $n = \pm 1$  one obtains

$$\begin{aligned} f_{\hat{\mathbf{b}}}^{(E)} &= -E_{\hat{\mathbf{k}}} \frac{(4b^2 + \mathcal{I}^\lambda\mathcal{I}^\kappa)\partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^s\mathcal{I}^\kappa \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}}}{4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa} \longrightarrow -E_{\hat{\mathbf{k}}} \left( \frac{1}{\mathcal{I}^+} \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \frac{\mathcal{I}^\kappa}{4b^2} \left( \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \frac{1}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} \right) \right), \\ f_{\hat{\mathbf{c}}}^{(E)} &= -E_{\hat{\theta}} \frac{\mathcal{I}^\kappa(\mathcal{I}^s\partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^+ \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}})}{4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa} \longrightarrow -E_{\hat{\theta}} \frac{N\mathcal{I}^\kappa}{4b^2} \left( \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \frac{1}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} \right), \\ f_z^{(E)} &= -E_{\hat{\theta}} \frac{2b(\mathcal{I}^s\partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \mathcal{I}^+ \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}})}{4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa} \longrightarrow -E_{\hat{\theta}} \frac{N}{2b} \left( \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} + \frac{1}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} \right). \end{aligned} \quad (72)$$

The far right shows the monolayer case  $N = \pm 1$ . The result (72) is the solution to all orders in  $(\ell k_F)^{-1}$ . The expansion can be carried out by expanding the denominator in  $\mathcal{I}/b$ . In the monolayer case  $N = \pm 1$  the denominator simplifies as  $|M| = 4b^2\mathcal{I}^+$  due to  $\mathcal{I}^\lambda = \mathcal{I}^+$  and  $\mathcal{I}^s \equiv N\mathcal{I}^+$ , therefore no expansion is possible. Consequently, contributions beyond the leading order correction will be absent in the monolayer case. Our monolayer result has a structure similar to that of equations (13) and (14) in Trushin *et al* [21], however, up to the sign of the  $(1/k)f_{\hat{\mathbf{b}}}^{\text{eq}}$  part. The sign difference, which originates from the sign of  $E_{\hat{\theta}}(N/k)f_{\hat{\mathbf{b}}}$  in the left-hand side of (65), will determine the sign of  $\sigma^{\text{II}}$  to be introduced below.

The charge current  $\mathbf{j}$  in momentum space, see equation (8), is in the graphene case ( $\epsilon_0 = 0$ ) given by

$$\mathbf{j}(\mathbf{k}) = 2\hat{\mathbf{k}}f_{\hat{\mathbf{b}}}\partial_k b + 2\hat{\theta}\mathbf{f}_{\hat{\mathbf{c}}}\frac{Nb}{k} \longrightarrow 2v_F(\hat{\mathbf{k}}f_{\hat{\mathbf{b}}} + N\hat{\theta}\mathbf{f}_{\hat{\mathbf{c}}}) \quad (73)$$

with the monolayer case  $N = \pm 1$  to the right. With  $\int_{\theta} \hat{\mathbf{k}}E_{\hat{\mathbf{k}}} = \int_{\theta} \hat{\theta}E_{\hat{\theta}} = \mathbf{E}/2$  one obtains the current in real space

$$\mathbf{j} = \int_{\mathbf{k}} \mathbf{j}(\mathbf{k}) = (\sigma^{\text{I}} + \sigma^{\text{II}})\mathbf{E}. \quad (74)$$

The conductivity is given by the contributions

$$\begin{aligned} \sigma^{\text{I}} &= - \int \frac{k \, dk}{2\pi} \frac{(4b^2 + \mathcal{I}^\kappa\mathcal{I}^\lambda)\partial_k b + \mathcal{I}^\kappa\mathcal{I}^s \frac{Nb}{k}}{4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa} \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} \longrightarrow - \frac{v_F}{2\pi} \int k \, dk \left( \frac{1}{\mathcal{I}^+} + \frac{\mathcal{I}^\kappa\mathcal{I}^+}{2b^2} \right) \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} \\ \sigma^{\text{II}} &= - \int \frac{dk}{2\pi} N \frac{\mathcal{I}^\kappa\mathcal{I}^s\partial_k b + \mathcal{I}^\kappa\mathcal{I}^+ \frac{Nb}{k}}{4b^2\mathcal{I}^+ + \mathcal{I}^+\mathcal{I}^\lambda\mathcal{I}^\kappa - (\mathcal{I}^s)^2\mathcal{I}^\kappa} f_{\hat{\mathbf{b}}}^{\text{eq}} \longrightarrow - \frac{v_F}{2\pi} \int dk \frac{\mathcal{I}^\kappa}{2b^2} f_{\hat{\mathbf{b}}}^{\text{eq}}, \end{aligned} \quad (75)$$

where for the monolayer case to the far right it was used that  $\partial_k b = b/k = v_F$  for all  $k$ . Because of  $\mathcal{I}_{-N}^s = -\mathcal{I}_N^s$  the conductivity is invariant with the sign of  $N$ .

As a part of  $\sigma^{\text{I}}$  we recognize the Drude contribution  $\sigma_0 = - \int (k \, dk/2\pi)(\partial_k b/\mathcal{I}^+) \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} = \ell k_F/4\pi$ . The contributions  $\sigma^{\text{II}}$  and  $\delta\sigma^{\text{I}} = \sigma^{\text{I}} - \sigma_0$  are quantum corrections, both of order  $(\ell k_F)^{-1}$  and for  $|N| \leq 2$  containing also higher powers of  $(\ell k_F)^{-1}$ . Notice that there is no contribution of the order  $(\ell k_F)^0$ .

At  $T = 0$  one has from (67) that  $f_{\mathbf{b}}^{\text{eq}} = -\frac{1}{2}\Theta(k - k_{\text{F}})$  and  $\partial_k f_{\mathbf{b}}^{\text{eq}} = -\frac{1}{2}\delta(k - k_{\text{F}})$ . The conductivity including the leading quantum correction  $\sim(\ell k_{\text{F}})^{-1}$  (for general  $N$  obtained by a truncated expansion of the denominator in (75)) becomes

$$\begin{aligned}\sigma^{\text{I}} &= \sigma_0 \left( 1 + \frac{\mathcal{I}_{\text{F}}^{\kappa}(\mathcal{I}_{\text{F}}^{\text{s}})^2}{4b_{\text{F}}^2\mathcal{I}_{\text{F}}^+} + \frac{N\mathcal{I}^{\kappa}\mathcal{I}^{\text{s}}}{4b_{\text{F}}v_{\text{F}}k_{\text{F}}} \right) + \mathcal{O} \left( \left( \frac{1}{\ell k_{\text{F}}} \right)^2 \right) \longrightarrow \sigma_0 \left( 1 + \frac{\mathcal{I}_{\text{F}}^{\kappa}\mathcal{I}_{\text{F}}^+}{2b_{\text{F}}^2} \right), \\ \sigma^{\text{II}} &= \frac{1}{4\pi} \int_{k_{\text{F}}}^{\infty} dk \left( \frac{N\mathcal{I}^{\kappa}\mathcal{I}^{\text{s}}\partial_k b}{4b^2\mathcal{I}^+} + \frac{N^2\mathcal{I}^{\kappa}}{4bk} \right) + \mathcal{O} \left( \left( \frac{1}{\ell k_{\text{F}}} \right)^2 \right) \longrightarrow \frac{1}{8\pi} \int_{b_{\text{F}}}^{\infty} db \frac{\mathcal{I}^{\kappa}}{b^2},\end{aligned}\tag{76}$$

where we write out the monolayer ( $N = \pm 1$ ) result to the far right. With real spin and valley degeneracies included, the conductivity of graphene is  $\sigma_{\text{graphene}} = 4(\sigma^{\text{I}} + \sigma^{\text{II}})$ . The leading correction depends on  $\mathcal{I}^{\kappa}$  but not on  $\mathcal{I}^{\lambda}$ . Thus the difference in  $\mathcal{I}^{\kappa}$ —that is the one in  $\mathcal{J}_z[f_z]$ —is the one that is crucial for the discrepancy between approaches.

The leading corrections are positive within all the approaches. When we later include principal value terms this will no longer be the case.

For screened charged impurities  $W(k, \Delta\theta) = 2\pi n_{\text{imp}}(2k \sin(|\Delta\theta|/2) + k_{\text{TF}})^{-2}$  the integral in  $\sigma^{\text{II}}$  is convergent. For point-like impurities  $K(k, \Delta\theta) = (k/2\pi v)W_0$  with  $W_{\mathbf{k}\mathbf{k}'} = W_0 = \text{const} \propto n_{\text{imp}}$  the integral for  $\sigma^{\text{II}}$  has a logarithmic divergence in the monolayer case (since  $\mathcal{I} \propto k/v = k/v_{\text{F}}$ ) unless an ultraviolet cut-off is introduced. Let us nonetheless make the observation that  $\mathcal{I}^+ = K/4$  and  $\mathcal{I}^- = 3K/4$ . Given a cut-off, the leading quantum correction is larger by a factor of 3 with the approach G1wGKBA ( $\mathcal{I}^{\kappa} = \mathcal{I}^-$ ) compared to the approaches G1wAA/vN/NSO ( $\mathcal{I}^{\kappa} = \mathcal{I}^+$ ). Other approaches lie midway between these two results.

For point-like impurities in the multilayer case  $|N| \geq 2$  all the approaches coincide because

$$\mathcal{I}^+ = \frac{1}{2}K = \tilde{\mathcal{I}}^+ = \mathcal{I}^- \tag{77}$$

hence  $\mathcal{I}^+ = \mathcal{I}^{\lambda} = \mathcal{I}^{\kappa} =: \mathcal{I}$ . Furthermore  $\mathcal{I}^{\text{s}} = 0$ . With  $b = \alpha k^N$  and  $\mathcal{I} = \frac{1}{2}K = (k^{2-N}/4\pi N\alpha)W_0$  the  $T = 0$  limit of the untruncated form (75) is easy to carry out. The result is (here with  $e$  and  $\hbar$  reintroduced)

$$\sigma^{\text{I}} = \sigma_0 \quad \sigma^{\text{II}} = \frac{e^2}{2h} \frac{N^2}{4(|N| - 1)} \arctan \frac{|N|}{2\ell k_{\text{F}}}. \tag{78}$$

All integrals converge without any ultraviolet cut-off. The  $N = 2$  case of (78) was worked out in collaboration with Trushin *et al*, see [10].

The treatment in this section would until equation (75) also hold for the density matrix  $\rho$ , provided that  $\rho_{\mathbf{b}}^{\text{eq}}$  is independent of  $\hat{\mathbf{k}}$  and that  $\rho_{\mathbf{c}}^{\text{eq}} = \rho_z^{\text{eq}} = 0$ . The difference would come in the last step (76). If the difference between  $\rho_{\mathbf{b}}^{\text{eq}}$  and  $f_{\mathbf{b}}^{\text{eq}}$  is of order  $V^r$ ,  $r \leq 4$ , it could in principle change the value or the order of the leading quantum correction.

## 7. AC response

For an ac field  $\mathbf{E}(t) = e^{i\omega t}\mathbf{E}$  one obtains with the Ansatz  $f_{\mathbf{k}}^{(E)}(t) = e^{i\omega t}f_{\mathbf{k}}^{(E)}$  the Boltzmann equation

$$e^{i\omega t}(i\omega f_{\mathbf{k}}^{(E)} + i[H, f_{\mathbf{k}}^{(E)}] + \mathbf{E} \cdot \partial_{\mathbf{k}} f_{\mathbf{k}}^{\text{eq}} - \mathcal{J}[f_{\mathbf{k}}^{(E)}]) = 0 \tag{79}$$

from which the Drude result (63) is modified into

$$\sigma_0(\omega) := \frac{v_F k_F}{4\pi(\tau_{\text{trF}}^{-1} + i\omega)} = \frac{\ell k_F}{4\pi(1 + i\omega\tau_{\text{trF}})}. \quad (80)$$

In the coherent treatment of spin of section 6 the term  $i\omega f^{(E)} e^{i\omega t}$  enters as a diagonal matrix  $i\omega \mathbf{1}_4$  in equation (69), i.e. we obtain the ac result from the dc result for the  $n = \pm 1$  Fourier components with the substitutions

$$\mathcal{I}^+ \rightarrow \mathcal{I}^+ + i\omega, \quad \mathcal{I}^\kappa \rightarrow \mathcal{I}^\kappa + i\omega, \quad \mathcal{I}^\lambda \rightarrow \mathcal{I}^\lambda + i\omega, \quad \mathcal{I}^s \rightarrow \mathcal{I}^s. \quad (81)$$

Since the Boltzmann equation (79) with  $\omega \neq 0$  is no longer real, the  $n = -1$  component of the solution is no longer obtained by simply complex conjugating the  $n = +1$  component of the solution. The correct  $n = -1$  component is obtained by carrying out the substitution (81) *after* the complex conjugation. This is the same as carrying out the substitution in the full dc solution where the two Fourier components have already been added up. With (81) the dc result (72) is modified into the ac result

$$\begin{aligned} f_{\hat{b}}^{(E)} &= -E_{\hat{k}} \frac{1}{|M|} \left( [4b^2 + (\mathcal{I}^\lambda + i\omega)(\mathcal{I}^\kappa + i\omega)] \partial_k f_{\hat{b}}^{\text{eq}} + \mathcal{I}^s [\mathcal{I}^\kappa + i\omega] \frac{1}{k} f_{\hat{b}}^{\text{eq}} \right) \longrightarrow -E_{\hat{k}} \partial_k f_{\hat{b}}^{\text{eq}} \frac{1}{i\omega}, \\ f_{\hat{c}}^{(E)} &= -E_{\hat{\theta}} \frac{1}{|M|} (\mathcal{I}^\kappa + i\omega) \left( \mathcal{I}^s \partial_k f_{\hat{b}}^{\text{eq}} + [\mathcal{I}^+ + i\omega] \frac{1}{k} f_{\hat{b}}^{\text{eq}} \right) \longrightarrow -E_{\hat{\theta}} \frac{1}{k} f_{\hat{b}}^{\text{eq}} \frac{i\omega}{4b^2 - \omega^2}, \\ f_z^{(E)} &= -E_{\hat{\theta}} \frac{1}{|M|} 2b \left( \mathcal{I}^s \partial_k f_{\hat{b}}^{\text{eq}} + [\mathcal{I}^+ + i\omega] \frac{1}{k} f_{\hat{b}}^{\text{eq}} \right) \longrightarrow -E_{\hat{\theta}} \frac{1}{k} f_{\hat{b}}^{\text{eq}} \frac{2b}{4b^2 - \omega^2}, \end{aligned} \quad (82)$$

with the determinant  $|M|$  also shifted according to (81). We complemented this with the pure sample limits ( $W_{kk'} \rightarrow 0$ ) to the far right.

Ac terms are derived from dc terms by replacing a real quantity  $\mathcal{I}$  by an imaginary quantity  $i\omega$ . Thus the real frequency dependent contributions in  $\sigma(\omega)$  step up or down in even powers of  $\omega/\mathcal{I}$ , whereas an odd power would be needed to derive a  $(\ell k_F)^0$  correction in  $\text{Re } \sigma(\omega)$  from the dc result  $\sigma_{\text{Drude}} \sim \ell k_F$  or its dc corrections  $\sim (\ell k_F)^{-1}$ . According to this argument, there are no corrections  $(\ell k_F)^0$  to  $\text{Re } \sigma(\omega)$ . This result should be contrasted with the frequency dependent corrections of order  $(\ell k_F)^0$  found by Culcer *et al* (equations (31) and (27) in [22]).

For further details, see appendix D.

## 8. First quantum correction with principal value terms included

In this section we include the principal value terms and recalculate the first quantum correction to the conductivity, this time in a recursive solution in the spirit of [22]. The recursion is only taken to order  $(\ell k_F)^0$  in the distribution function, but could in principle be reiterated to access terms of order  $(\ell k_F)^{-1}$  and higher as discussed in appendix E. However, the structure of the recursive setting makes it clearer why the  $(\ell k_F)^0$  correction goes only into  $f_z$ , whereas  $f_{\hat{b}}$ ,  $f_{\hat{c}}$ —and by consequence the current—get no contribution if principal value terms are neglected. When the latter are included the recursive setting clearly shows why  $f_{\hat{b}}$  and  $f_{\hat{c}}$  then can get corrections already of the order  $(\ell k_F)^0$ .

We will start by giving the physical reason for taking principal value terms seriously in our semiclassical kinetic equations. General collision integrals derived within a quantum coherent approach typically contain principal value terms (a.k.a. reaction terms, off-shell terms, off-pole terms) alongside the delta function terms (a.k.a. elastic terms, on-shell terms, pole terms). The delta functions convey the sharpness in energy of the idealized semiclassical quasiparticles. The quasiparticles are the almost free particles that will distribute themselves according to the Fermi–Dirac distribution in equilibrium, whereas the electrons due to the interaction will be given by a distribution with fatter tails [30]. The principal value terms are reminiscent of the quantum coherent nature of the underlying particles and capture the deviation from the classical point-like ‘billiard ball’ picture conveyed by the fully semiclassical (i.e. quantum incoherent) Boltzmann equation. One such example is the principal value terms related to the quickly decaying coherences coming from the redressing of the quasiparticles within the interaction radius [30]. The corresponding decay time (the collision time, the spent within the interaction radius) is in the kinetic regime, by assumption much shorter than the relaxation time (roughly  $\tau_{tr}$ ), hence the electron quickly recovers its asymptotic quasiparticle nature after one collision on its way to the next. In the spectral function the off-pole part is the broad background around the quasiparticle peak [58]. For spinless electrons there are ways of separating the off-pole part from the quantum kinetic equation, with the remainder becoming the standard Boltzmann equation for the quasiparticles [30].

The electron–hole coherence (or spin-coherence), too, is a deviation from the fully semiclassical particle picture, in this case not because of interaction effects but because of the Zitterbewegung due to the spin–orbit coupling. It is therefore no surprise that a spin–orbit coupling contributes with its own principal value terms adding to those related to the quasiparticle redressing. However, this time we do not want to separate out the principal values in deriving a Boltzmann type equation since the Zitterbewegung is known to be inherent in the asymptotic free particle. When we want to derive a kinetic equation while keeping track of electron–hole coherence effects, we should therefore keep the corresponding principal value terms. To our knowledge this physical motivation has not been given before in the graphene context nor in related fields (e.g. spin Hall effect, anomalous Hall effect). The only reference we know of that treats principal value terms due to spin (although not spin–orbit coupling) is the Green’s function derivation by Langreth and Wilkins [56] of a Boltzmann equation for electrons interacting with localized spins. There the principal value terms are found to give important renormalizations.

The technical problem with including principal value terms is that the two momenta  $\mathbf{k}$  and  $\mathbf{k}'$  in the collision integral are no longer confined to sit on the same surface. This is in contrast with the previous situation which allowed us to unplug the Fourier coefficients  $f_{rn}(k)$  from the integrals, of which the remainder become matrix elements like  $\mathcal{I}^\pm$  etc. (The problem of solving the Boltzmann equation to all orders in  $(\ell k_F)^{-1}$  then reduced to a matrix inversion.) With the principal value terms we have to confront difficult integro-differential equations. In [20] an analytical solution to all orders in  $(\ell k_F)^{-1}$  was obtained for point-like impurities. The solution for screened charged impurities is still unknown and will be addressed here within the recursive scheme. It happens that we do not run into the problem of finding unknowns inside of the integrals  $\mathcal{J}^P$  with principal values. Therefore, no simplifying assumption about the potential is needed.

From the principal value terms in (58) we find in the case G1wAA/vN/NSO

$$\begin{aligned}
 \mathcal{J}_0^P &= 0, & \mathcal{J}_b^P &= - \int_{k'} W_{kk'} \left( -\frac{\sin N\Delta\theta}{2\pi\Delta b} + \frac{\sin N\Delta\theta}{2\pi(b+b')} \right) \Delta f_z, \\
 \mathcal{J}_{\hat{c}}^P &= - \int_{k'} W_{kk'} \left( -\frac{\cos^2(N\Delta\theta/2)}{\pi\Delta b} - \frac{\sin^2(N\Delta\theta/2)}{\pi(b+b')} \right) \Delta f_z, \\
 \mathcal{J}_z^P &= - \int_{k'} W_{kk'} \left\{ \frac{\cos^2(N\Delta\theta/2)\Delta f_{\hat{c}} + (\sin N\Delta\theta/2)(f_{\hat{b}} + f_{\hat{b}'})}{\pi\Delta b} \right. \\
 &\quad \left. + \frac{\sin^2(N\Delta\theta/2)(f_{\hat{c}} + f_{\hat{c}'}) - (\sin N\Delta\theta/2)\Delta f_{\hat{b}}}{\pi(b+b')} \right\}.
 \end{aligned} \tag{83}$$

For a comparison with Auslender *et al* [20], see appendix C. The case G1wGKBA is obtained by simply exchanging the principal values  $1/\Delta b$  and  $1/(b+b')$ , as can be seen in (58). Decomposing  $\mathcal{J}^P = \mathcal{J}^{PX} + \mathcal{J}^{PY}$  for G1wGKBA into parts even and odd, respectively, under  $\Delta b \leftrightarrow b+b'$  we have

$$\begin{aligned}
 \mathcal{J}_b^{PX} &= 0, & \mathcal{J}_b^{PY} &= - \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \sin N\Delta\theta f'_z, \\
 \mathcal{J}_{\hat{c}}^{PX} &= + \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} + \frac{1}{\Delta b} \right) \Delta f_z, \\
 \mathcal{J}_{\hat{c}}^{PY} &= + \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \cos N\Delta\theta \Delta f_z, \\
 \mathcal{J}_z^{PX} &= - \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} + \frac{1}{\Delta b} \right) (f_{\hat{c}} - \cos N\Delta\theta f'_{\hat{c}} + \sin N\Delta\theta f'_{\hat{b}}), \\
 \mathcal{J}_z^{PY} &= - \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) (\cos N\Delta\theta f_{\hat{c}} - f'_{\hat{c}}).
 \end{aligned} \tag{84}$$

The corresponding expressions for the other approaches considered in the paper are obtained by multiplying the  $\mathcal{J}^{PX}$  and  $\mathcal{J}^{PY}$  components, respectively, with  $+1$ ,  $-1$  or  $0$  according to (49).

For the same reasons as before only the Fourier components  $n = \pm 1$  of the nonequilibrium part  $f^{(E)}$  can be nonzero. Therefore one only needs to consider

$$\begin{aligned}
 \mathcal{J}_{b1}^{PX} &= 0 & \mathcal{J}_{b1}^{PY} &= +i \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \sin N\Delta\theta \sin \Delta\theta f'_{z1}, \\
 \mathcal{J}_{\hat{c}1}^{PX} &= + \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} + \frac{1}{\Delta b} \right) (f_{z1} - \cos \Delta\theta f'_{z1}), \\
 \mathcal{J}_{\hat{c}1}^{PY} &= + \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \cos N\Delta\theta (f_{z1} - \cos \Delta\theta f'_{z1}), \\
 \mathcal{J}_{z1}^{PX} &= - \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} + \frac{1}{\Delta b} \right) (f_{\hat{c}1} - \cos N\Delta\theta \cos \Delta\theta f'_{\hat{c}1} - i \sin N\Delta\theta \sin \Delta\theta f'_{\hat{b}1}), \\
 \mathcal{J}_{z1}^{PY} &= - \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) (\cos N\Delta\theta f_{\hat{c}1} - \cos \Delta\theta f'_{\hat{c}1}).
 \end{aligned} \tag{85}$$

Both in (84) and in (85) have we left out all terms that vanish due to the assumed symmetry  $W(-\Delta\theta) = W(\Delta\theta)$  of the potential. We will see below that for the calculation

of the first quantum correction one only needs to know  $\mathcal{J}_z^P[f_{\hat{b}}]$  and  $\mathcal{J}_{\hat{b}}^P[f_z]$ , that is

$$\begin{aligned}\mathcal{J}_{z1}^{\text{PX}}[f_{\hat{b}}] &= i \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} + \frac{1}{\Delta b} \right) \sin N\Delta\theta \sin \Delta\theta f'_{\hat{b}1}, \\ \mathcal{J}_{\hat{b}1}^{\text{PY}}[f_z] &= i \int_{k'} \frac{W_{kk'}}{2\pi} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \sin N\Delta\theta \sin \Delta\theta f'_{z1}.\end{aligned}\quad (86)$$

We can already at this stage extract some general conclusions for the multilayer case  $|N| \neq 1$  with point-like impurities. The trivial vanishing of the angular integral in (86) will imply below that principal value terms do not contribute to order  $(\ell k_F)^0$ . Nor do they contribute to order  $(\ell k_F)^{-1}$  (see appendix E). Combining (49) with the fact the terms  $\mathcal{J}^{\text{PY}}$  in (85) vanish trivially, we conclude that principal value terms do not contribute to any order for the G2 approaches. The integrals  $\mathcal{J}^{\text{PX}}$  vanish non-trivially in the special case  $|N| = 2$ , in which case the principal value vanishes in all approaches (including the density matrix approach [10]). To the orders to which principal value terms do not contribute, the quantum corrections are given by the treatment in section 6. For the monolayer case principal value terms can contribute to the correction  $\sim(\ell k_F)^0$  in all approaches, with the trivial exception of G2wSKBA.

The Boltzmann equation for  $\mathbf{f}^{(E)}$  (we henceforth drop the superscript  $(E)$ ) can be written as

$$\mathcal{D} = \mathcal{S}[\mathbf{f}] + \mathcal{J}^\delta[\mathbf{f}] + \mathcal{J}^P[\mathbf{f}], \quad (87)$$

where  $\mathcal{D}$  is the driving term with

$$\begin{pmatrix} \mathcal{D}_{\hat{b}} \\ \mathcal{D}_{\hat{c}} \\ \mathcal{D}_z \end{pmatrix} = \begin{pmatrix} E_{\hat{k}} \partial_k f_{\hat{b}}^{\text{eq}} \\ E_{\hat{\theta}} \frac{N}{k} f_{\hat{b}}^{\text{eq}} \\ 0 \end{pmatrix}, \quad (88)$$

$\mathcal{S}[\mathbf{f}]$  is the spin-precession term

$$\begin{pmatrix} \mathcal{S}_{\hat{b}}[\mathbf{f}] \\ \mathcal{S}_{\hat{c}}[\mathbf{f}] \\ \mathcal{S}_z[\mathbf{f}] \end{pmatrix} = \begin{pmatrix} 0 \\ -2bf_z \\ 2bf_{\hat{c}} \end{pmatrix}, \quad (89)$$

and the functionals  $\mathcal{J}^\delta$  and  $\mathcal{J}^P$  are read off from (65), (66), (83) and the remarks below (83). A more informative way of writing equation (87) is

$$\begin{aligned}\mathcal{D}_{\hat{b}} &= 0 + \mathcal{J}_{\hat{b}}^\delta[f_{\hat{b}}, f_{\hat{c}}] + \mathcal{J}_{\hat{b}}^P[f_z] & \mathcal{D}_{\hat{c}} &= \mathcal{S}_{\hat{c}}[f_z] + \mathcal{J}_{\hat{c}}^\delta[f_{\hat{b}}, f_{\hat{c}}] + \mathcal{J}_{\hat{c}}^P[f_z] \\ 0 &= \mathcal{S}_z[f_{\hat{c}}] + \mathcal{J}_z^\delta[f_z] + \mathcal{J}_z^P[f_{\hat{b}}, f_{\hat{c}}].\end{aligned}\quad (90)$$

For notational simplicity we now prefer to see the expansion of  $f$  in orders of  $(\ell k_F)^{-1}$  as one in powers of  $W_{kk'}$ , i.e.

$$f = f^{(-1)} + f^{(0)} + f^{(1)} + \dots \quad (91)$$

with  $f^{(n)} \propto W^n \propto (\ell k_F)^{-n}$ . Here  $f^{(-1)} \propto W^{-1}$  is the lowest order result that yields the Drude conductivity. Notice that the functionals  $\mathcal{J}[f]$  increase the power in  $W$  by one whereas the action of  $\mathcal{S}[f]$  is neutral in powers of  $W$ . Therefore, the two latter equations do not allow  $f_{\hat{c}}$  and  $f_z$  to have a lowest order component  $W^{-1}$ , since  $\mathcal{S}[f^{(-1)}]$  would return a term of order  $W^{-1}$ , which could not be matched by any of the other terms  $\mathcal{D}$  ( $\sim W^0$ ) and

$\mathcal{J}[f]$  ( $\sim W^0$  and higher). The absence of  $\mathcal{S}_{\hat{\mathbf{b}}}$  in the first equation (the diagonal components do not precess) is what allows only  $f_{\hat{\mathbf{b}}}$  to have a term of order  $W^{-1}$ . Solving  $\mathcal{D}_{\hat{\mathbf{b}}} = \mathcal{J}_{\hat{\mathbf{b}}}[f_{\hat{\mathbf{b}}}^{(-1)}]$  ( $\sim W^0$ ), yields  $f_{\hat{\mathbf{b}}}^{(-1)} = -E_{\hat{\mathbf{k}}}\tau_{\text{tr}}\partial_k f^{\text{eq}}$ .

The components  $f^{(0)}$  are found by solving the system

$$\begin{aligned} 0 &= 0 + \mathcal{J}_{\hat{\mathbf{b}}}^{\delta}[f_{\hat{\mathbf{b}}}^{(0)}, f_{\hat{\mathbf{c}}}^{(0)}] + \mathcal{J}_{\hat{\mathbf{b}}}^{\text{P}}[f_z^{(0)}] & (\sim W^1) \\ \mathcal{D}_{\hat{\mathbf{c}}} &= \mathcal{S}_{\hat{\mathbf{c}}}[f_z^{(0)}] + \mathcal{J}_{\hat{\mathbf{c}}}^{\delta}[f_{\hat{\mathbf{b}}}^{(-1)}] + 0 & (\sim W^0) \\ 0 &= \mathcal{S}_z[f_{\hat{\mathbf{c}}}^{(0)}] + 0 + \mathcal{J}_z^{\text{P}}[f_{\hat{\mathbf{b}}}^{(-1)}] & (\sim W^0) \end{aligned} \quad (92)$$

where  $f_{\hat{\mathbf{b}}}^{(-1)}$  is known. The two latter equations constitute a closed set, which allows us to first find  $f_{\hat{\mathbf{c}}}^{(0)}$  and  $f_z^{(0)}$ . Only the known component  $f_{\hat{\mathbf{b}}}^{(-1)}$  goes into the principal value part. The system of equation is solved as in the previous sections by Fourier decomposition and matrix inversion,

$$\begin{aligned} \begin{pmatrix} \frac{iN\mathcal{E}^*}{2k} f_{\hat{\mathbf{b}}}^{\text{eq}} \\ 0 \end{pmatrix} &= \begin{pmatrix} 0 & -2b \\ 2b & 0 \end{pmatrix} \begin{pmatrix} f_{\hat{\mathbf{c}}1}^{(0)} \\ f_{z1}^{(0)} \end{pmatrix} + \begin{pmatrix} i\mathcal{I}^{\text{s}} f_{\hat{\mathbf{b}}1}^{(-1)} \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \mathcal{J}_{z1}^{\text{P}}[f_{\hat{\mathbf{b}}}^{(-1)}] \end{pmatrix} \\ \Rightarrow \begin{pmatrix} f_{\hat{\mathbf{c}}1}^{(0)} \\ f_{z1}^{(0)} \end{pmatrix} &= \begin{pmatrix} -\frac{1}{2b} \mathcal{J}_{z1}^{\text{P}}[f_{\hat{\mathbf{b}}}^{(-1)}] \\ -\frac{1}{2b} \frac{i\mathcal{E}^*}{2} \left( \frac{N}{k} f_{\hat{\mathbf{b}}}^{\text{eq}} + \frac{\mathcal{I}^{\text{s}}}{\mathcal{I}^{\text{+}}} \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} \right) \end{pmatrix}. \end{aligned} \quad (93)$$

Notice that if we discard the principal value terms  $\mathcal{J}^{\text{P}}$  we find that  $f_{\hat{\mathbf{c}}}^{(0)} = 0$ , which using the first equation in (92) implies  $f_{\hat{\mathbf{b}}}^{(0)} = 0$ . This is exactly what the solution (71) tells us: there is no  $W^0$  correction (i.e.  $(\ell k_{\text{F}})^0$  correction) to the conductivity in (76); only  $f_z$  obtains a contribution to order  $W^0$ . The last line of (93) indeed corresponds to  $f_z$  in (71).

Including principal value terms yields a nonzero  $f_{\hat{\mathbf{c}}}^{(0)}$ . It also gives a nonzero  $f_{\hat{\mathbf{b}}}^{(0)}$  according to the first equation in (92),

$$0 = \mathcal{J}_{\hat{\mathbf{b}}}^{\delta}[f_{\hat{\mathbf{b}}}^{(0)}, f_{\hat{\mathbf{c}}}^{(0)}] + \mathcal{J}_{\hat{\mathbf{b}}}^{\text{P}}[f_z^{(0)}] = -\mathcal{I}^{\text{+}} f_{\hat{\mathbf{b}}1}^{(0)} - i\mathcal{I}^{\text{s}} f_{\hat{\mathbf{c}}1}^{(0)} + \mathcal{J}_{\hat{\mathbf{b}}1}^{\text{P}}[f_z^{(0)}]. \quad (94)$$

Nonzero in-plane components

$$f_{\hat{\mathbf{b}}1}^{(0)} = i \frac{\mathcal{I}^{\text{s}}}{2b\mathcal{I}^{\text{+}}} \mathcal{J}_{z1}^{\text{P}}[f_{\hat{\mathbf{b}}}^{(-1)}] + \frac{1}{\mathcal{I}^{\text{+}}} \mathcal{J}_{\hat{\mathbf{b}}1}^{\text{P}}[f_z^{(0)}], \quad f_{\hat{\mathbf{c}}1}^{(0)} = -\frac{1}{2b} \mathcal{J}_{z1}^{\text{P}}[f_{\hat{\mathbf{b}}}^{(-1)}] \quad (95)$$

result in a correction to the conductivity. In particular, this correction is of order  $(\ell k_{\text{F}})^0$  since the components in (95) are of order  $(\ell k_{\text{F}})^0$ .

A closer inspection shows that  $f_{\hat{\mathbf{b}}1}^{(0)}/\mathcal{E}^*$  is real and  $f_{\hat{\mathbf{c}}1}^{(0)}/\mathcal{E}^*$  is imaginary, as was the case in (71). This implies (consult equations (72) and (68)) that  $f_{\hat{\mathbf{b}}}^{(0)} = E_{\hat{\mathbf{k}}} 2f_{\hat{\mathbf{b}}1}^{(0)}/\mathcal{E}^*$  and  $f_{\hat{\mathbf{c}}}^{(0)} = E_{\hat{\theta}} 2f_{\hat{\mathbf{c}}1}^{(0)}/i\mathcal{E}^*$ . The first quantum correction  $\delta\sigma$  to the conductivity is therefore for arbitrary  $N$  given by

$$\mathbf{E}\delta\sigma = 2 \int_{\mathbf{k}} \left( \hat{\mathbf{k}} f_{\hat{\mathbf{b}}}^{(0)} \partial_k b + \hat{\theta} f_{\hat{\mathbf{c}}}^{(0)} \frac{Nb}{k} \right) = 2\mathbf{E} \int \frac{k dk}{2\pi} \left( \frac{f_{\hat{\mathbf{b}}1}^{(0)}}{\mathcal{E}^*} \partial_k b + \frac{f_{\hat{\mathbf{c}}1}^{(0)}}{i\mathcal{E}^*} \frac{Nb}{k} \right) \propto (\ell k_{\text{F}})^0. \quad (96)$$

From (95) one obtains the first quantum correction as a sum of the contributions

$$\begin{aligned}\delta\sigma^X &= -2 \int \frac{k dk}{2\pi} \frac{1}{i\mathcal{E}^*2b} \left( \frac{\mathcal{I}_k^s}{\mathcal{I}_k^+} \partial_k b + \frac{Nb}{k} \right) \mathcal{J}_{z1}^P[f_{\hat{b}}^{(-1)}], \\ \delta\sigma^Y &= +2 \int \frac{k dk}{2\pi} \frac{\partial_k b}{\mathcal{E}^* \mathcal{I}_k^+} \mathcal{J}_{b1}^P[f_z^{(0)}].\end{aligned}\quad (97)$$

This can be written as

$$\begin{aligned}\delta\sigma^X &= +\frac{1}{2\pi} \int \frac{k dk}{2\pi} \left( \frac{\mathcal{I}_k^s}{\mathcal{I}_k^+} \partial_k b + \frac{Nb}{k} \right) \int \frac{k' dk'}{2\pi} \frac{1}{\mathcal{I}_{k'}^+} \partial_{k'} f_{\hat{b}}^{\text{eq}'} \int_{\theta'} W_{kk'\Delta\theta} \frac{\sin N\Delta\theta \sin \Delta\theta}{b^2 - b'^2}, \\ \delta\sigma^Y &= -\frac{1}{2\pi} \int \frac{k dk}{2\pi} \frac{1}{\mathcal{I}_k^+} \partial_k b \int \frac{k' dk'}{2\pi} \left( \frac{\mathcal{I}_{k'}^s}{\mathcal{I}_{k'}^+} \partial_{k'} f_{\hat{b}}^{\text{eq}'} + \frac{N}{k'} f_{\hat{b}}^{\text{eq}'} \right) \int_{\theta'} W_{kk'\Delta\theta} \frac{\sin N\Delta\theta \sin \Delta\theta}{b^2 - b'^2},\end{aligned}\quad (98)$$

where we introduced the notation  $W_{kk'\Delta\theta} := W_{\mathbf{k}\mathbf{k}'}$ . It is easily seen that for point-like impurities the angular integral vanishes trivially for  $|N| \geq 2$ . For further results on point-like impurities see appendix E.

At zero temperature the correction (98) can be written as

$$\begin{aligned}\delta\sigma^X &= -\frac{k_F}{8\pi^2 \mathcal{I}_F^+} \int \frac{k dk}{2\pi} \left( \frac{\mathcal{I}_k^s}{\mathcal{I}_k^+} \partial_k b + \frac{Nb}{k} \right) \int_{\theta'} W_{kk_F\Delta\theta} \frac{\sin N\Delta\theta \sin \Delta\theta}{b^2 - b_F^2} \\ \delta\sigma^Y &= +\frac{k_F \mathcal{I}_F^s}{8\pi^2 \mathcal{I}_F^+} \int \frac{k dk}{2\pi} \frac{1}{\mathcal{I}_k^+} \partial_k b \int_{\theta'} W_{kk_F\Delta\theta} \frac{\sin N\Delta\theta \sin \Delta\theta}{b^2 - b_F^2} \\ &\quad + \frac{N}{8\pi^2} \int \frac{k dk}{2\pi} \frac{1}{\mathcal{I}_k^+} \partial_k b \int_{k_F}^{\infty} dk' \int_{\theta'} W_{kk'\Delta\theta} \frac{\sin N\Delta\theta \sin \Delta\theta}{b^2 - b'^2}\end{aligned}\quad (99)$$

and in the monolayer case  $N = \pm 1$  this can be simplified to (with  $\partial_k b = b/k = v_F$  and writing  $\mathcal{I}_k^+ = (k/4\pi v_F) \int_{\theta'} W_{kk\Delta\theta} \sin^2 \Delta\theta$ )

$$\begin{aligned}\delta\sigma^X &= -\frac{e^2}{2\pi\hbar} \frac{\int dk (k/(k^2 - k_F^2)) \int_{\theta'} W_{kk_F\Delta\theta} \sin^2 \Delta\theta}{\int_{\theta'} W_{k_F k_F \Delta\theta} \sin^2 \Delta\theta}, \\ \delta\sigma^Y &= +\frac{e^2}{2\pi\hbar} \int dk \frac{k_F}{k^2 - k_F^2} \frac{\int_{\theta'} W_{kk_F\Delta\theta} \sin^2 \Delta\theta}{\int_{\theta'} W_{kk\Delta\theta} \sin^2 \Delta\theta} \\ &\quad + \frac{e^2}{2\pi\hbar} \int dk \int_{k_F}^{\infty} dk' \frac{1}{k^2 - k'^2} \frac{\int_{\theta'} W_{kk'\Delta\theta} \sin^2 \Delta\theta}{\int_{\theta'} W_{kk\Delta\theta} \sin^2 \Delta\theta},\end{aligned}\quad (100)$$

where we reintroduced  $e$  and  $\hbar$ . For point-like impurities these integrals are easily evaluated:

$$\begin{aligned}\delta\sigma^X / \frac{e^2}{2\pi\hbar} &= -\int_0^{k_\Lambda} dk \frac{k}{k^2 - k_F^2} = -\log \frac{k_\Lambda}{k_F} + \mathcal{O}\left(\left(\frac{k_F}{k_\Lambda}\right)^2\right), \\ \delta\sigma^Y / \frac{e^2}{2\pi\hbar} &= \int_0^{k_\Lambda} dk \frac{k_F}{k^2 - k_F^2} + \int_0^{k_\Lambda} dk \int_{k_F}^{k_\Lambda} dk' \frac{1}{k^2 - k'^2} = -\frac{\pi^2}{8} + \mathcal{O}\left(\left(\frac{k_F}{k_\Lambda}\right)^2\right),\end{aligned}\quad (101)$$

where an ultraviolet cut-off  $k_\Lambda \gg k_F$  was introduced. Notice that only  $\delta\sigma^X$  is ultraviolet divergent.

The total quantum correction is  $\delta\sigma = 4(\pm\delta\sigma^X \pm \delta\sigma^Y)$  with relative prefactors (possibly zero) given by (49) for the different approaches. Notice that the leading quantum

correction will not be positive in all approaches, in contrast to the situation in section 6. For point-like impurities, in particular, we find

		$\delta\sigma/\frac{2e^2}{\pi h}$
vN & NSO &	G1 GKBA	$-\log\frac{k_\Lambda}{k_F} - \frac{\pi^2}{8}$
	G1 AA	$-\log\frac{k_\Lambda}{k_F} + \frac{\pi^2}{8}$
	G1 SKBA	$-\log\frac{k_\Lambda}{k_F}$
	G2 GKBA	$-\frac{\pi^2}{8}$
	G2 AA	$+\frac{\pi^2}{8}$
	G2 SKBA	0.

(102)

The leading quantum correction is ultraviolet divergent for all the G1 approaches, including the density matrix approaches, whereas it is convergent for the G2 approaches. Furthermore, only the approach G2wAA gives a positive correction, namely

$$\delta\sigma = \frac{\pi e^2}{4h} \quad (\text{G2wAA}). \quad (103)$$

In the Boltzmann regime  $\ell k_F \gg 1$  this is a small positive shift to the much bigger Drude conductivity  $4\sigma_0 = (2e^2/h)\ell k_F = (e^2/h)(8v_F^2/n_{\text{imp}}V_0^2)$  for a constant potential  $V_{\mathbf{k}\mathbf{k}'} = V_0$ . We mention that for screened charge impurities ultraviolet divergences are absent.

To obtain a contribution of order  $(\ell k_F)^{-1}$ , which should explain the initial onset of convexity in the conductivity as one approaches the Dirac regime, one iterates this recursive procedure, see appendix E. It is once again the case that one only needs to insert known distribution functions into the integrals containing principal values. Therefore an analytical solution is possible although increasingly cumbersome. By considering the expansion parameter  $(\mathcal{I}^+ + i\omega)/b$  the iterative procedure can be repeated in order to find corrections to the ac conductivity. The ac analog is obtained with the substitutions (81).

The result (103) applies to point-like impurities. Strictly speaking the assumption of negligible inter-valley scattering should break down, and it is questionable if the results can be used to discuss graphene experiments. This caveat does not apply either for topological insulators with only one Dirac cone (see the end of section 1), or, of course, to numerical simulations of graphene including only one cone. Our main drive, however, is graphene with screened charged impurities and, in particular, monolayer graphene with the screening parameter  $q_s := k_{\text{TF}}/k_F \approx 3.2$ , relevant for samples on silicon-oxide substrates. We will assume that this is already long-range enough for inter-valley scattering to be of secondary importance. In that case the two-valley results and one-valley results should be roughly the same, and we can discuss the former, relying on results for the latter. We can now speculate that our leading quantum correction could be one of the contributions to the residual conductivity observed in the experiments of Chen *et al* [13]. We plan to return to the quantitative analysis in future work. However, already here we can draw some qualitative conclusions based on the present section and recalling facts from section 2. The value of the correction can only depend on the dimensionless parameter  $q_s$ , which for monolayers is independent of  $k_F$  and hence independent of the electron density. This leads to a rigid vertical shift of the Drude conductivity as a function of electron density, as illustrated in figure 1. The size of this shift depends only on natural constants and the dielectric constant present in  $k_{\text{TF}}$ . Thus, the quantum correction could depend on the dielectric environment of the monolayer graphene sample.

We have given a quantitative evaluation for the correction  $(\ell k_F)^0$  in the limit  $q_s \rightarrow \infty$ , because here this limit coincides with that of point-like impurities. (This was the situation for the Drude conductivity (see section 2). However, there the absolute scaling with  $k_F$  in the scattering times was relevant, in contrast to the case of the correction (100)). We have also evaluated the shift (100) in the opposite limit  $q_s = 0 < 1$  of an unscreened Coulomb interaction. We find the corrections to be ultraviolet divergent and we find the sign of  $\sigma^Y$  to be the opposite. However, since  $q_s \approx 3.2 > 1$ , we expect the limit  $q_s \rightarrow \infty$  to be the more relevant limit. Therefore we expect also for the realistic value  $q_s = 3.2$  to encounter the case that only the one approach G2wAA gives a positive value, and that value is likely to be close to (103). In the case where inter-valley scattering is negligible with  $q_s = 3.2$ , this value should then also be relevant for the two-valley situation and thus for graphene experiments.

Puddle formation due to charge inhomogeneities leads to a variation in the Fermi level, see e.g. [50]. However, our shift should be insensitive at least to small variations as it is independent of the Fermi level. In the case where the impurities sit at a non-negligible average distance  $d$  from the graphene plane this introduces a second dimensionless parameter  $k_F d$ , which depends on the density. In this scenario  $\delta\sigma$  becomes density dependent and the shift is no longer rigid. However, in the Fermi momentum range  $\ell^{-1} \ll k_F \ll d^{-1}$ , which is the range where the Drude conductivity should be linear, the effect on the statements above should be negligible. Thus, the residual conductivity we make predictions for should be fitted only from the ‘strictly’ linear part of the Boltzmann conductivity.

Next we discuss the leading quantum correction (99) in multilayers. We have shown that for point-like impurities it vanishes trivially. Thus—referring to section 2—we expect the correction to vanish close to the Dirac point. However, the interesting limit is the one far away from the Dirac point, where (99) is all that remains of the studied quantum corrections. Here, it is more relevant to compare with the unscreened Coulomb interaction. Irrespective of whether or not the correction is finite in this limit, it becomes doubtful that our analysis is still valid in this regime. The kinetic approach assumes that the collision time set by the range of the potential is short compared to the relaxation time  $\tau_{\text{tr}}$ . For point-like impurities this is certainly the case, whereas for an unscreened Coulomb potential it is highly questionable. For a long-range potential it certainly becomes important to take into account mean-field effects and their renormalizations of the free drift, which we have neglected. These issues have been discussed in the context of strongly interacting spinless Fermi systems, see [30]. At the moment we do not know how to generalize these issues to systems with non-trivial spin. Therefore, we cannot say much about whether there could be non-vanishing effects due to electron–hole coherence for multilayers with charged impurities. Since finite effects of electron–hole coherence far away from the Dirac regime are very counterintuitive, we find it likely that in a proper treatment of the multilayer problem they would vanish at very high densities. However, in monolayers we expect such effects to survive, as we come to next.

Monolayer graphene stands out in many respects and comes with many surprises compared to multilayer graphene because of the linear dispersion and the unit winding number  $|N| = 1$ . (See also [24, 27] on why  $|N| = 1$  is special.) We saw already in section 2 that monolayers are different to multilayers and 2DEGs when it comes to how the screening depends on the electron density. Therefore we should not straight away

discard as unphysical the finding of finite effects of electron–hole coherences far away from the Dirac regime, although we expect no such effects in general and, in particular, not in multilayers. In both monolayers and multilayers the Fermi surface—and therefore the number of electrons contributing to a nonequilibrium response—grows linearly with  $k_F$ . A Kubo formula for the conductivity (see e.g. equation (2) in [10]) disfavors matrix elements between states with a large energy separation. The Zitterbewegung contribution from each electron would therefore be suppressed by the large energy denominators  $1/[\epsilon^+(k_F) - \epsilon^-(k_F)] \sim k_F^{-N}$ . In the case of multilayers this suppression wins over the increasing density of states as  $k_F$  increases. However, in the monolayer case the two effects compensate each other, therefore a finite effect of Zitterbewegung at large energy splitting is not inconceivable.

One might worry about the electron–hole coherent effects being negligible compared to weak localization corrections. However, this is not necessarily the case, at least in idealized situations, as should be clear from recent calculations [10], where the analytically found electron–hole coherent conductivity stays very close to the numerically exact value, with the small rather constant discrepancy probably due to weak localization. Nor should the electron–hole coherent shift in monolayers be negligible in the residual conductivity, since we find it to be of the order of one quantum of conductance. Further, the different leading order quantum corrections can be cleanly separated and therefore treated independently. From the kinetic equation treatment of weak localization in [49] we see that the weak localization correction takes only the Drude response part of the nonequilibrium Green’s function as its input and not the full Green’s function including contributions of higher order in  $(\ell k_F)^{-1}$ . Thus, like the Drude response, the weak localization correction should be independent of the choice of formalism. Therefore, we believe that the weak localization correction and our  $(\ell k_F)^0$  correction can be cleanly separated, and that the issue of formalism affects only the latter.

## 9. Conclusions and outlook

In this paper we investigated different derivations of semiclassical but spin-coherent Boltzmann equations in a case where differences could matter, namely in the electron–hole coherence originated quantum corrections to the Drude conductivity for 2d Dirac electrons, as encountered in graphene, or in the surface states of 3d topological insulators such as  $\text{Bi}_{1-x}\text{Sb}_x$ ,  $\text{Bi}_2\text{Te}_3$ ,  $\text{Sb}_2\text{Te}_3$  and  $\text{Bi}_2\text{Se}_3$ . With a few exceptions we find these quantum corrections to be highly sensitive to the approach. We find the leading quantum correction in monolayer graphene to be particularly interesting as a litmus test, and suggest that a precise determination of this contribution from numerics or experiments might single out a unique approach. This sensitivity has motivated us to search for an Ansatz that provides the link between a quantum Liouville equation derivation and a Green’s function derivation, that we find to differ with existing approaches. The simple structures of the derived collision integral in their most general form makes this search unambiguous. We have found the missing link, at least for the case of impurity interactions in the lowest Born approximation, and propose a novel Ansatz (AA) of a simple but counterintuitive form that, to our knowledge, has not been studied before.

On a more technical level we pointed out that the fact that the pseudospin–orbit coupling is the dominant term in the Hamiltonian is essential for the differences to become important. The fact that spin–orbit coupling constitutes the entire kinetic part in the

graphene case simplifies the collision integral considerably and makes an analytic solution possible. The analytic treatment becomes non-trivial due to the presence of principal value terms. We discussed the physical origin of these terms and explained why one, also in our kinetic description, should take them seriously. In addition, we showed how to deal with them for arbitrary scalar impurity potentials, at least for not too long-ranged potentials. We kept the winding number of the spin-orbit coupling general in order to address single layer graphene as well as multilayer graphene.

We found that the first quantum correction depends both on the chosen formalism as well as on whether or not principal value terms are included. With principal value terms neglected, the leading quantum correction is found to be of order  $(\ell k_F)^{-1}$ . When they are included, and do not vanish, the leading quantum correction is of order  $(\ell k_F)^0$ . An electron-hole coherence originated quantum correction  $\sim(\ell k_F)^0$  would be a counterintuitive result as it implies that electron-hole coherence effects could remain finite even far away from the Dirac regime. We discussed why such a result in the case of monolayers is not absurd, although surprising. In multilayers, on the other hand, we do not expect such a result, and indeed for point-like impurities the correction  $\sim(\ell k_F)^0$  vanishes trivially. For screened charged impurities one encounters the situation that the potential approaches the opposite limit—the unscreened Coulomb potential—when one increases the density. Since the kinetic analysis in this paper disregarded renormalization effects of the free drift, our analysis should break down when the quasiparticle spends a sizable fraction of its time within the interaction range of the impurities. Therefore, we do not attempt to evaluate the correction  $\sim(\ell k_F)^0$  for multilayers with charged impurities in the high density limit where the screening is weak.

We argued that the shift in monolayers due to electron-hole coherences should only depend on the dielectric constant through the dimensionless parameter  $q_s$ . We also argued that the evaluated leading correction for monolayers with point-like impurities should be closely related to the one relevant to experiments, since for monolayers on silicon-oxide substrates the screening parameter  $q_s \approx 3.2$  is bigger than one and therefore more related to the limit  $q_s = \infty$  than to the limit  $q_s = 0$ . Such a shift could be one of the contributions in the residual conductivity observed in recent experiments [13]. Our contribution  $\delta\sigma$ , given in (100), depends crucially on the approach to deriving collision integrals. With a precise measurement of the residual conductivity and a precise knowledge of other contributions (e.g. weak (anti-)localization) that one would need to take into account, monolayer graphene would offer an unprecedented setting for experimentally singling out one among all the approaches restudied or introduced in the present paper. In a comparison with numerics one would of course have an even more controlled setting. We plan to address the actual quantitative analysis and comparison with experiments and numerics in future work.

The observed residual conductivity is positive. If also the contribution from electron-hole coherences was determined to be positive, this would pick the approach called G2wAA as the unique alternative. Interestingly, this contains the Ansatz AA, which is one of our original contributions. In such a case, the electron-hole coherence effects of graphene would require a kinetic equation that even in principle could not have been derived with existing theory.

The more technical work on the Ansatz and the introduction of the generalized Kadanoff-Baym Ansatz (GKBA) [38] was prompted by the study of high-field transport

for spinless electrons, see [39]. It would be interesting to study the consequences of our Ansatz on transport beyond linear response. The two Ansätze certainly differ when electron–hole coherent effects are important, but it is not known to us if there is a difference for spinless electrons in strong electric fields.

As already mentioned in section 1 we believe that all the presented approaches might still have to be refined, in particular for the case of weakly screened impurities, which is relevant for multilayers with charged impurities and at high Fermi momentum. The elaborate literature on Boltzmann transport for spinless electrons offers two clear directions for improvement that we believe could also be important for the quantum corrections due to the pseudospin–orbit interaction.

- (1) A proper accounting for all terms that could contribute to first order in the electric field. For example taking into account that also the non-interacting response functions  $G^{0R}$  and  $G^{0A}$  are modified by the electric field and that the gradient expansion of the self-energy terms to first order includes electric field contributions in a gauge invariant formulation. In the context of spin–orbit interactions this was discussed recently in [27]. For electron systems with a trivial spin index these issues have been discussed for more than two decades in the context of high-electric-field transport, see [39] for a review. See also [47, 57].
- (2) A proper extraction of the quasiparticle part  $f$  in the kinetic equation for  $\rho$  (or  $G^<$ ) and a proper incorporation of renormalizations of the free drift. In the process one unveils the qualitative difference between the electron distribution function  $\rho$  and the quasiparticle distribution  $f$ . The difference appears as a wavefunction renormalization factor and as an extra term containing principal values. The latter term is related to the quickly decohering off-shell motion from the quasiparticle redressing within the interaction radius. For single-band electrons these issues have also been discussed for some two decades, for example in the context of Boltzmann treatments of Fermi systems with strong two-body interactions (for an extensive review we refer to [30], for the context of impurities, see [59]). Here it becomes important to recognize that  $f^{\text{eq}} = f_{\text{FD}} \neq \rho^{\text{eq}}$ . Only by properly separating out the coherences related to the quasiparticle redressing can one in a controlled way extract a Boltzmann equation that one solves by linearizing around an equilibrium described by the Fermi–Dirac distribution  $f_{\text{FD}}$ .

It is an open question as to how one can generalize these issues to situations with interband coherences. However, already at the level of treatment given in the present paper we believe the discussed approach to be very promising for understanding electron–hole coherent effects in the conductivity in graphene, with the recent results in [10] being one example of this promise.

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## Appendix A. Translating evolution operators into Green's functions

With  $H_{\mathbf{k}} = \epsilon_{0\mathbf{k}} + \boldsymbol{\sigma} \cdot \mathbf{b}_{\mathbf{k}}$  we notice that

$$\begin{aligned}
 \int_0^\infty dt e^{-\eta t} e^{-iH_{\mathbf{k}}t} f e^{iH_{\mathbf{k}'}t} &= \int_0^\infty dt e^{-\eta t} e^{-i(\epsilon_0 - \epsilon_0')t} \\
 &\times \sum_s \frac{e^{-isbt} + s\boldsymbol{\sigma} \cdot \hat{\mathbf{b}} e^{-isbt}}{2} f \sum_{s'} \frac{e^{is'b't} + s'\boldsymbol{\sigma} \cdot \hat{\mathbf{b}}' e^{is'b't}}{2} \\
 &= \int_0^\infty dt e^{-\eta t} \sum_{ss'} e^{-i(\epsilon_0 + sb - \epsilon_0' - s'b')t} S f S' = \sum_{ss'} S f S' \frac{1}{\eta + i(\epsilon - \epsilon')} \\
 &= \int \frac{d\omega}{2\pi} \sum_{ss'} \frac{S}{\omega + i\eta - \epsilon} f \frac{S'}{\omega - i\eta - \epsilon'} = \int \frac{d\omega}{2\pi} G_{\mathbf{k}}^{0R} f G_{\mathbf{k}'}^{0A}.
 \end{aligned} \tag{A.1}$$

## Appendix B. Details on the anti-ordered Kadanoff–Baym Ansatz

In [38] the correlator  $G^<$  is divided into the auxiliary correlators

$$G^{<r}(t_1, t_2) = \theta(t_1 - t_2) G^<(t_1, t_2), \quad G^{<a}(t_1, t_2) = \theta(t_2 - t_1) G^<(t_1, t_2). \tag{B.1}$$

By acting on  $G^{<r}$  with  $(G^R)^{-1}$  from the left, using the generalized Kadanoff–Baym equation (42) and then acting on the result with  $G^R$  from the left one arrives at

$$\begin{aligned}
 G^{<r}(t_1, t_2) &= iG^R(t_1, t_2) G^<(t_2, t_2) + \int_{t_2}^{t_1} dt \int_{-\infty}^{t_2} dt' G_{t_1 t_2}^R \Sigma_{t't_2}^R G_{t't_2}^< + G_{t_1 t_2}^R \Sigma_{t't_2}^< G_{t't_2}^A, \\
 G^{<a}(t_1, t_2) &= -iG^<(t_1, t_1) G^A(t_1, t_2) + \int_{-\infty}^{t_1} dt \int_{t_1}^{t_2} dt' G_{t_1 t_2}^R \Sigma_{t't_2}^< G_{t't_2}^A + G_{t_1 t_2}^< \Sigma_{t't_2}^A G_{t't_2}^A.
 \end{aligned} \tag{B.2}$$

We complemented this with the corresponding result for  $G^{<a}$  with  $(G^A)^{-1}$  and  $G^A$  instead acting from the right. The first terms to the right sum up to the GKBA. The integrals are correction terms that fulfil several natural criteria. (1) On the time-diagonal  $t_1 = t_2$  they vanish, making the GKBA exact. (2) No integrals stretch to  $t = +\infty$ , i.e. the result respects the causality of the Kadanoff–Baym equations. (3) One can derive the same equations for  $G^>$ , i.e. particle–hole symmetry remains. (4) The spectral identity  $G^< + G^> = i(G^R - G^A)$  is still satisfied.

The solution can be used to determine  $G^<$  iteratively to the desired precision. Thus, the GKBA can be seen as the first term in an expansion in the interaction strength. However, in [38] it is noted that, on top of that, the arguments of the self-energies  $\Sigma_{t't'}$  run over disjoint intervals, which makes the integrals even smaller and relates to the collision time  $\tau_0 (\ll \tau_{\text{tr}})$ , the small time the particles spends within the interaction radius.

We now copy this treatment but act with the response functions from the opposite sides (i.e. acting on  $G^{<r}$  with  $(G^R)^{-1}$  from the right using the generalized Kadanoff–Baym equation (42) and then acting on the result with  $G^R$  again from the right). This gives us instead

$$\begin{aligned}
 G^{<r}(t_1, t_2) &= iG^<(t_1, t_1) G^R(t_1, t_2) + \int^{t_1} dt' (G^R \Sigma^< + G^< \Sigma^A - G^{<r} \Sigma^R)_{t_1 t'} G_{t' t_2}^R, \\
 G^{<a}(t_1, t_2) &= -iG^A(t_1, t_2) G^<(t_2, t_2) + \int^{t_2} dt G_{t_1 t}^A (\Sigma^R G^< + \Sigma^< G^A - \Sigma^A G^{<a})_{t t_2}.
 \end{aligned} \tag{B.3}$$

The criteria (1)–(4) are still satisfied. Note in particular that the causality is respected. However, the result is a bit more complicated, and this time the variables  $t$  and  $t'$  in the self-energies no longer run over disjoint time intervals. Our conclusion is that the expansion can still be seen as one in the interaction strength but no longer as one in the collision time. However, when comparing Boltzmann equations derived using Green's function techniques with one derived with a Liouville equation approach, it is sufficient to be consistent to the given order of the interaction.

### Appendix C. Comparison with the Boltzmann equation of Auslender and Katsnelson

The Boltzmann equation for the Dirac cone K was derived by Auslender and Katsnelson [20] with the NSO formalism. For comparison we are going to translate our Boltzmann equation into theirs. (Similar to us they do not consider the terms with  $\delta(b + b')$ .) In [20] the Boltzmann equation is written for the quantities  $D := 2f_0 - 1$ ,  $N := 2f_{\hat{b}} + 1$  (not be confused with our winding number  $N$ ) and  $g := f_z - if_{\hat{c}}$ . In terms of these we obtain

$$\begin{aligned}
 \mathbf{E} \cdot \partial_{\mathbf{k}} D &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \cos^2 \frac{\Delta\theta}{2} \Delta D, \\
 \mathbf{E} \cdot \partial_{\mathbf{k}} N + 2 \frac{E_{\hat{\theta}}}{k} \text{Im } g &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \left\{ \delta(\Delta b) \left( \cos^2 \frac{\Delta\theta}{2} \Delta N + \sin \Delta\theta \text{Im } g' \right) \right. \\
 &\quad \left. + \left( \frac{\sin \Delta\theta}{\pi \Delta b} - \frac{\sin \Delta\theta}{\pi(b + b')} \right) \text{Re } g' \right\}, \\
 \mathbf{E} \cdot \partial_{\mathbf{k}} g - i \frac{E_{\hat{\theta}}}{2k} (N - 1) - i 2bg &= - \int_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'} \left\{ \delta(\Delta b) \left( \cos^2 \frac{\Delta\theta}{2} \Delta g - i \frac{\sin \Delta\theta}{4} N' \right) \right. \\
 &\quad \left. + \left( \frac{i \cos^2(\Delta\theta/2) \Delta g + (\sin \Delta\theta/4) N'}{\pi \Delta b} + \frac{i \cos^2(\Delta\theta/2) \Delta g + (\sin \Delta\theta/4) N'}{\pi(b + b')} \right) \right\}. \tag{C.1}
 \end{aligned}$$

Linearizing (e.g.  $D = D_0 + \delta D(E)$ ) the equations in the electric field and comparing with (47), (51) and (52) in [20] we recognize all the terms. Apart from some minor differences in prefactors the main difference is the  $\delta D$  in equation (52) is in our case  $\delta N$ . In our Boltzmann equation the electron density  $f_0$  (i.e.  $D$ ) decouples from the spin density  $\mathbf{f}$  (i.e.  $N$  and  $g$ ). This decoupling is also found in [22].

### Appendix D. On the ac response with principal value terms neglected

In this appendix we concentrate on the monolayer case  $N = \pm 1$ . With (81) the determinant becomes

$$\begin{aligned}
 |M| &= 4b^2(\mathcal{I}^+ + i\omega) + (\mathcal{I}^+ + i\omega)^2(\mathcal{I}^\kappa + i\omega) - (\mathcal{I}^s)^2(\mathcal{I}^\kappa + i\omega) \\
 &= 4b^2(\mathcal{I}^+ + i\omega) \left( 1 + \frac{i\omega(2\mathcal{I}^+ + i\omega)(\mathcal{I}^\kappa + i\omega)}{4b^2(\mathcal{I}^+ + i\omega)} \right). \tag{D.1}
 \end{aligned}$$

The conductivity derived from (82) is given by

$$\begin{aligned}\sigma^{\text{I}}(\omega) &= -v_{\text{F}} \int \frac{k \, dk}{2\pi} \frac{1}{|M|} \partial_k f_{\hat{\mathbf{b}}}^{\text{eq}} (4b^2 + (\mathcal{I}^\kappa + i\omega)(2\mathcal{I}^+ + i\omega)), \\ \sigma^{\text{II}}(\omega) &= -v_{\text{F}} \int \frac{k \, dk}{2\pi} \frac{1}{k|M|} f_{\hat{\mathbf{b}}}^{\text{eq}} (\mathcal{I}^\kappa + i\omega)(2\mathcal{I}^+ + i\omega).\end{aligned}\tag{D.2}$$

Under the assumption  $\omega, \mathcal{I} \ll b_{\text{F}} \equiv |\mu|$  (here  $T = 0$ ) the Fermi surface contribution  $\sigma^{\text{I}}$  can be expanded in  $\omega/|\mu|$  and  $\mathcal{I}/|\mu|$  with  $|M|^{-1} \approx (1/4b^2(\mathcal{I}^+ + i\omega))(1 - (i\omega(2\mathcal{I}^+ + i\omega)(\mathcal{I}^\kappa + i\omega)/4b^2(\mathcal{I}^+ + i\omega)))$  to yield the leading order correction

$$\sigma^{\text{I}}(\omega) \approx \sigma_0(\omega) \left( 1 + \frac{\mathcal{I}_{\text{F}}^+(2\mathcal{I}_{\text{F}}^+ + i\omega)(\mathcal{I}_{\text{F}}^\kappa + i\omega)}{4|\mu|^2(\mathcal{I}_{\text{F}}^+ + i\omega)} \right).\tag{D.3}$$

As already visible in (82), in the pure limit  $\mathcal{I} \rightarrow 0$ , there are no corrections in  $\sigma^{\text{I}}$  to  $\sigma_0 = -i(|\mu|/4\pi\omega)$ . For  $\mathcal{I} \neq 0$ ,  $\sigma^{\text{I}}$  has, in contrast to the dc results of the last section, a correction of order  $(\ell k_{\text{F}})^0$ . However, this correction only affects the inductive part  $\text{Im} \sigma^{\text{I}}$ . For  $\omega \ll \mathcal{I}^+$  and for  $\kappa = +$  we find that  $\sigma^{\text{I}}(\omega) \approx \sigma_0 + (1/8\pi\ell k_{\text{F}}) - i(\omega/16\pi|\mu|)$ . For the contribution  $\sigma^{\text{II}}$  the above expansion of  $|M|^{-1}$  is allowed since  $b$  only sweeps the interval  $[|\mu|, \infty)$ . However, the integral is cumbersome. We only give the result in the clean limit  $\mathcal{I} = 0$ ,

$$\sigma^{\text{II}}(\omega) = -i\frac{\omega}{4\pi} \int_0^\infty db \frac{f_{\text{FD}}(b - \mu) - f_{\text{FD}}(-b - \mu)}{4b^2 - \omega^2} \stackrel{(T \rightarrow 0)}{=} i\frac{1}{32\pi} \ln \frac{2|\mu| + \omega}{2|\mu| - \omega} \approx i\frac{\omega}{32\pi|\mu|}.\tag{D.4}$$

In contrast to the corresponding result for  $\mathcal{I} \neq 0$ , this result does not diverge in the limit  $\omega \rightarrow 0$ .

## Appendix E. Details on a second iteration when principal value terms are included

In the second iteration the Boltzmann equation (90) reads

$$\begin{aligned}0 &= 0 + \mathcal{J}_{\hat{\mathbf{b}}}^\delta[f_{\hat{\mathbf{b}}}^{(1)}, f_{\hat{\mathbf{c}}}^{(1)}] + \mathcal{J}_{\hat{\mathbf{b}}}^{\text{P}}[f_z^{(1)}] && (\sim W^2) \\ 0 &= \mathcal{S}_{\hat{\mathbf{c}}}[f_z^{(1)}] + \mathcal{J}_{\hat{\mathbf{c}}}^\delta[f_{\hat{\mathbf{b}}}^{(0)}, f_{\hat{\mathbf{c}}}^{(0)}] + \mathcal{J}_{\hat{\mathbf{c}}}^{\text{P}}[f_z^{(0)}] && (\sim W^1) \\ 0 &= \mathcal{S}_z[f_{\hat{\mathbf{c}}}^{(1)}] + \mathcal{J}_z^\delta[f_z^{(0)}] + \mathcal{J}_z^{\text{P}}[f_{\hat{\mathbf{b}}}^{(0)}, f_{\hat{\mathbf{c}}}^{(0)}] && (\sim W^1).\end{aligned}\tag{E.1}$$

The driving terms that were still present in the first iteration—see equation (92)—are completely absent in the second and higher iterations. The components  $f_{\hat{\mathbf{b}}}^{(0)}$ ,  $f_{\hat{\mathbf{c}}}^{(0)}$  and  $f_z^{(0)}$ —which determined the correction of order  $(\ell k_{\text{F}})^0$  in the conductivity—are the known input in the Boltzmann equation (E.1) from which one then extracts the components  $f_{\hat{\mathbf{b}}}^{(1)}$ ,  $f_{\hat{\mathbf{c}}}^{(1)}$  and  $f_z^{(1)}$ . The latter components determine the correction of order  $(\ell k_{\text{F}})^{-1}$  in the conductivity.

We see that generally also the contribution of order  $(\ell k_{\text{F}})^{-1}$  depends on the principal value terms. However, their contribution vanishes again trivially in the case of point-like impurities together with  $|N| \neq 1$ , as already happens in the first recursion with the consequence that  $f_{\hat{\mathbf{b}}}^{(0)}$ ,  $f_{\hat{\mathbf{c}}}^{(0)}$  and the contribution  $\sim (\ell k_{\text{F}})^0$  to the conductivity are all

zero. For this case we immediately find  $f_{\hat{c}}^{(1)} = -\mathcal{S}_{z1}^{-1}[\mathcal{J}_z^\delta[f_z^{(0)}]] = \mathcal{I}^\kappa/2bf_z^{(0)}$  (see (69)) independent of principal value terms and therefore consistent with (71). In contrast,  $f_z^{(1)} = -\mathcal{S}_{\hat{c}1}^{-1}[\mathcal{J}_{\hat{c}}^P[f_z^{(0)}]]$  will depend on principal value terms. The pertinent expression for G1 wGKBA is given by

$$\mathcal{J}_{\hat{c}}^P[f_z] = \frac{1}{2\pi} + \int_{k'} W_{kk'} \left( \frac{\sin^2 N\Delta\theta/2}{\Delta b} + \frac{\cos^2 N\Delta\theta/2}{b+b'} \right) \Delta f_z, \quad (\text{E.2})$$

derived with  $\Delta b \leftrightarrow (b+b')$  from the result (83) for G1wAA/vN/NSO. For the comparison with other approaches according to (49) we decompose (E.2) into

$$\begin{aligned} \mathcal{J}_{\hat{c}1}^{\text{PX}}[f_z] &= \frac{1}{4\pi} \int_{k'} W_{kk'} \left( \frac{1}{\Delta b} + \frac{1}{b+b'} \right) (f_{z1} - e^{-i\Delta\theta} f'_{z1}), \\ \mathcal{J}_{\hat{c}1}^{\text{PY}}[f_z] &= \frac{1}{4\pi} \int_{k'} W_{kk'} \left( \frac{1}{b+b'} - \frac{1}{\Delta b} \right) \cos N\Delta\theta (f_{z1} - e^{-i\Delta\theta} f'_{z1}). \end{aligned} \quad (\text{E.3})$$

The contribution  $\mathcal{J}^{\text{PX}}$  does not vanish for  $|N| \neq 1$  whereas  $\mathcal{J}^{\text{PY}}$  does. From (49) we deduce that principal value terms in the approaches G1 (but not G2) can contribute to  $f_z^{(1)}$ . However, this does not help as this contribution is removed in the last step,

$$f_{\hat{b}}^{(1)} = -(\mathcal{J}_{\hat{b}}^\delta)^{-1} \left[ \mathcal{J}_{\hat{b}}^\delta[f_{\hat{c}}^{(1)}] + \mathcal{J}_{\hat{b}}^P[f_z^{(1)}] \right], \quad (\text{E.4})$$

since  $\mathcal{J}_{\hat{b}}^P[f_z^{(1)}]$  for  $|N| \neq 1$  vanishes trivially for the only nonzero Fourier components  $n = \pm 1$ .

We have understood that principal value contributions to  $f_z$  do not matter. Only if they appear in  $f_{\hat{c}}$  can there be a contribution to the current. Inspection of (83) shows that the only principal value terms that do not trivially remove the  $n = 1$  Fourier component in the case  $|N| \neq 1$  are the term  $\mathcal{J}_z^P[f_{\hat{c}}]$  and the already considered term  $\mathcal{J}_{\hat{c}}^P[f_z]$ . Thus  $\mathcal{J}_z^P[f_{\hat{c}}^{(1)}]$  could contribute to  $f_{\hat{c}}^{(2)}$ . In a third recursion, i.e. for quantum corrections of the order  $(\ell k_F)^{-2}$ , it is therefore possible that principal value terms contribute to the conductivity even in the case of point-like impurities in the multilayer case  $|N| \neq 1$ . The possibility of leaving out the principal value terms therefore requires further investigation.

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