

## Semiclassical theories of the anomalous Hall effect

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## TOPICAL REVIEW

# Semiclassical theories of the anomalous Hall effect

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## Abstract

Recently, the semiclassical theory of the anomalous Hall effect induced by the Berry curvature in Bloch bands has been introduced. The theory operates only with gauge invariant concepts that have a simple semiclassical interpretation and provides a clear distinction among various contributions to the Hall current. While the construction of such an approach to the anomalous Hall effect problem has been long sought, only the new semiclassical theory demonstrated the agreement with quantitative results of rigorous approaches based on the Green function techniques. The purpose of this work is to review the semiclassical approach including the early ideas and the recent achievements.

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## 1. Introduction

1 The anomalous Hall effect (AHE) is one of the most famous  
2 transport phenomena in magnetic materials. Unlike in  
3 paramagnets, the Hall resistance  $R_{xy}$  of a magnetic film has  
4 two contributions. One is usual, it is proportional to the applied  
5 magnetic field  $H$ . The other one is anomalous, it is observable  
6 only in a ferromagnetic state. The anomalous contribution  
7 is often proportional to the magnetization rather than to the  
8 applied magnetic field

$$6 \quad R_{xy} = r_0 H + r_a M, \quad (1)$$

9 where  $M$  is the magnetization of the sample,  $r_0$  and  $r_a$  are  
10 constants that characterize the strength of the standard and  
11 the anomalous Hall resistivities, respectively. The recent  
12 theoretical research demonstrated that the linear dependence  
13 on  $M$  in (1) is not universal and the Hall resistivity can  
14 show resonance features as a function of variable parameters,  
15 including the magnetization.

16 The practical interest in the AHE has continuously been  
17 driven by a difficulty to measure the carrier density in  
18 ferromagnets. Standard techniques based on measurements  
19 of the Hall conductivity are obstructed by the considerable  
20 anomalous contribution which can be much greater than the  
21 standard Hall conductivity. Recent advances in spintronics,  
22 especially the creation of new types of diluted magnetic  
23 semiconductors, revived interest in the AHE as a useful

tool to control spin-polarized currents and to characterize the magnetization. In addition, the recent theoretical interest has been fueled by the new interpretation of the anomalous Hall conductivity in terms of Berry phases and topological defects in the crystal band structure. Many theoretical constructions that usually had been considered of relevance mainly in high energy physics such as noncommuting coordinates and magnetic monopoles, became useful and even measurable in experiments on the AHE [1–4].

Despite the long history and the considerable practical importance, the theory of the anomalous Hall effect has remained controversial. The first steps to explain the AHE in ferromagnets were made more than 50 years ago. Since then many articles were published to correct previous mistakes and to suggest new explanations. Many of such efforts still were incomplete. While they resolved several pieces of the puzzle they also disregarded others. Sometimes distinct quantitative predictions followed from applications of different methods to the same model. Such controversy persists even at the present time. For example, there is a number of recent publications with contradictory quantitative predictions for the AHE in the Rashba 2D electron system [5–14]; although the issue has finally been resolved [13, 14].

Many aspects of the AHE have been extensively reviewed in the literature. The detailed up to date discussion of experiments with diluted magnetic semiconductors and the comparison with existing numerical and theoretical predictions can be found in recent reviews [15–18]. The modern topological interpretation of the AHE and the Kubo formula in terms of a magnetic monopole in the momentum space was reviewed in [19]. There are also much older introductions [20, 21], concentrated on the side-jump effect in III–V semiconductors, although many concepts, discussed there, have been strongly revised in recent years. The recent review of these older work, made in the same spirit, can also be found in [22] together with the discussion of results on the spin Hall effect.

Numerous efforts to design a rigorous semiclassical approach that would explain in simple terms all possible contributions to the anomalous Hall conductivity including disorder effects, however, still lack a detailed comparison in a single work. The goal of the present review is to fill this gap and to discuss in more detail the existing semiclassical theories, their advantages and limitations. We start with the earliest ideas introduced by Karplus, Luttinger and Smit and end with the most recent constructions that demonstrated the 1–1 agreement with the rigorous quantum mechanical techniques.

The structure of this review is the following. In the rest of the introduction in section 1.1, we recall the basic text book information about the semiclassical approach to conductivity calculations taking as an example free electrons interacting with elastic scatterers. In section 1.2, I remind several commonly known facts about Bloch bands and explain how the introduction of the band structure complicates the creation of the semiclassical theory of the transport, especially in the application to the AHE. In section 2, I discuss the forces driving the AHE and review the earliest theories, including the quantum analog of the Boltzmann equation applied by

Luttinger (section 2.1) and the introduction of noncommuting coordinates by Adams and Blount (section 2.2). In section 3, I proceed with more recent theories based on the gauge invariant formulation of the wavepacket dynamics and its Berry phase interpretation. In sections 3.1 and 3.2, I will review the application of this approach to the anomalous Nernst effect, the intrinsic contribution and the side-jump effect. Sections 4 and 5 are devoted to the rigorous semiclassical theory of the AHE, free of most limitations of previous approaches. In section 4, I discuss the rules that connect the scattering matrix with the classical concepts such as the scattering probability and the size of the coordinate shift at a scattering event. In section 5, I introduce the semiclassical Boltzmann equation and subsequently explain all important contributions to the Hall conductivity. There I will also discuss the strength of the AHE and comparisons with rigorous quantum mechanical approaches. Section 6 is the summary that discusses the present status of the theory and outlines possible future research directions.

### 1.1. Semiclassical approach to conductivity calculations

Quantitative estimates of the dc AHE by standard techniques based on the evaluation of Green functions and their products invariably involve long complex calculations. It is hard to achieve transparent interpretations; therefore theories of the AHE normally focus on particular simple model Hamiltonians and ignore many-body interactions apart from mean-field exchange potentials that encode the magnetic order. Even with these simplifications, the AHE theory remains difficult to develop.

One of the problems is the small magnitude of the AHE in comparison to the longitudinal conductivity. When considering the perturbative expansion of the conductivity in the weak disorder limit, the AHE contribution appears only in subdominant terms of higher powers in small parameters. Many standard approximations turn out to be no longer valid at these orders. Even a proper counting of relevant terms of a similar strength was a problem in many cases. Another difficulty is in the physical interpretation of conductivity contributions in the Kubo formula or in the Keldysh technique. Generally these rigorous quantum mechanical approaches operate with nongauge-invariant objects, such as off-diagonal elements of Green functions, of the density matrix or of the velocity operator, which only in the end are combined in the gauge invariant expression for the conductivity. Such calculations, while formally rigorous, hide the physical origin of elementary microscopic processes. This complicates the analysis and the bookkeeping of the relevant contributions.

The alternative approach is based on the classical Boltzmann equation applied to the electron transport [23–25]. It can be justified by the fact that in sufficiently clean materials one can look at the transport from the basis of wavepackets rather than Bloch waves. In the dilute disorder limit, a wavepacket is not destroyed during long time and behaves in many respects as a classical particle. One can trace the motion of the wavepacket in external fields and describe it in terms that have a clear meaning in classical physics.

In crystals, electrons cannot be considered as free particles because they strongly interact with a periodic crystal potential. As we will see in following sections this creates interesting ingredients in the wavepacket dynamics but initially, we will describe the semiclassical theory free of these complications assuming that electrons do not interact with the crystal potential and with each other [23]. The impurity free Hamiltonian of such an electron system has plain wave eigenstates

$$\psi_{\mathbf{k}}(\mathbf{r}, t) = \frac{1}{L^{D/2}} e^{i\mathbf{k}\cdot\mathbf{r} - i\frac{k^2}{2m}t}, \quad (2)$$

where  $L$  is the size of the system,  $D$  is its spatial dimension and  $k = |\mathbf{k}|$ . To construct a wavepacket with a well defined average momentum  $\mathbf{k}_c$ , plain waves (2) should be superposed with the envelope function  $a(\mathbf{k})$ , sharply peaked near the point  $\mathbf{k} = \mathbf{k}_c$  so that  $\int d^D\mathbf{k} |a(\mathbf{k})|^2 \mathbf{k} = \mathbf{k}_c$ , then the wavepacket vector can be written in the coordinate representation as follows:

$$\Psi_{\mathbf{k}_c}(\mathbf{r}, t) = \int \frac{d^D\mathbf{k}}{L^{D/2}} a(\mathbf{k}) \exp \left\{ i \left( \mathbf{k} \cdot \mathbf{r} - \frac{k^2 t}{2m} \right) \right\}. \quad (3)$$

The normalization condition requires that

$$\begin{aligned} \langle \Psi_{\mathbf{k}_c} | \Psi_{\mathbf{k}_c} \rangle &= \int d^D\mathbf{r} \Psi_{\mathbf{k}_c}^*(\mathbf{r}, t) \Psi_{\mathbf{k}_c}(\mathbf{r}, t) \\ &= \int d^D\mathbf{k} |a(\mathbf{k})|^2 = 1 \end{aligned} \quad (4)$$

and the index  $\mathbf{k}_c$  tells that the wavepacket has this average momentum, namely, switching to the momentum representation one can find that

$$\begin{aligned} \mathbf{k}_c &= \langle \Psi_{\mathbf{k}_c} | \hat{\mathbf{k}} | \Psi_{\mathbf{k}_c} \rangle = \int d^D\mathbf{k} \int d^D\mathbf{k}' a(\mathbf{k}) a^*(\mathbf{k}') \langle \mathbf{k}' | \hat{\mathbf{k}} | \mathbf{k} \rangle \\ &= \int d^D\mathbf{k} |a(\mathbf{k})|^2 \mathbf{k}. \end{aligned} \quad (5)$$

The velocity of the free wavepacket center of mass can be derived as follows:

$$\begin{aligned} \dot{\mathbf{r}}_c &= \frac{d}{dt} \langle \Psi_{\mathbf{k}_c} | \hat{\mathbf{r}} | \Psi_{\mathbf{k}_c} \rangle = \frac{d}{dt} \left\{ \int \frac{d^D\mathbf{r}}{L^D} \int d^D\mathbf{k} \int d^D\mathbf{k}' \right. \\ &\quad \left. \times a(\mathbf{k}) a^*(\mathbf{k}') e^{-i\mathbf{k}'\cdot\mathbf{r}} \left( \mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \right) e^{i\frac{(k')^2 t}{2m} - i\frac{k^2 t}{2m}} \right\} \\ &= \frac{d}{dt} \left\{ \int d^D\mathbf{k} \int d^D\mathbf{k}' a(\mathbf{k}) a^*(\mathbf{k}') \right. \\ &\quad \left. \times \left( \int \frac{d^D\mathbf{r}}{L^D} e^{-i\mathbf{k}'\cdot\mathbf{r}} \left( -i \frac{\partial}{\partial \mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \right) \right) e^{i\frac{(k')^2 t}{2m} - i\frac{k^2 t}{2m}} \right\} \\ &= \frac{d}{dt} \left\{ \int d^D\mathbf{k} \int d^D\mathbf{k}' a^*(\mathbf{k}') \right. \\ &\quad \left. \times \delta(\mathbf{k} - \mathbf{k}') e^{i\frac{(k')^2 t}{2m}} i \frac{\partial}{\partial \mathbf{k}} [a(\mathbf{k}) e^{-i\frac{k^2 t}{2m}}] \right\} \\ &= \frac{d}{dt} \left\{ \int d^D\mathbf{k} |a(\mathbf{k})|^2 \frac{\mathbf{k}t}{m} \right\} \\ &\quad + \frac{d}{dt} \left\{ \int d^D\mathbf{k} a(\mathbf{k})^* \left( \frac{-i\partial}{\partial \mathbf{k}} a(\mathbf{k}) \right) \right\} = \frac{\mathbf{k}_c}{m}. \end{aligned} \quad (6)$$

In the external uniform electric field, the Hamiltonian operator is  $\hat{H} = \hat{k}^2/2 + e\mathbf{E}\cdot\hat{\mathbf{r}}$  and the average of the momentum

is changing with time

$$\begin{aligned} \dot{\mathbf{k}}_c &= \frac{d}{dt} \langle \Psi_{\mathbf{k}_c} | \hat{\mathbf{k}} | \Psi_{\mathbf{k}_c} \rangle_{\mathbf{E}} \\ &= \frac{d}{dt} \left\{ \int d^D\mathbf{k} \int d^D\mathbf{k}' a(\mathbf{k}) a^*(\mathbf{k}') \langle \mathbf{k}' | e^{i\hat{H}t} \hat{\mathbf{k}} e^{-i\hat{H}t} | \mathbf{k} \rangle \right\} \\ &= \int d^D\mathbf{k} \int d^D\mathbf{k}' a(\mathbf{k}) a^*(\mathbf{k}') \\ &\quad \times \langle \mathbf{k}' | [\hat{\mathbf{k}}, -ie\mathbf{E}\cdot\hat{\mathbf{r}}] | \mathbf{k} \rangle = -e\mathbf{E}, \end{aligned} \quad (7)$$

where  $\hat{\mathbf{k}}$  and  $\hat{\mathbf{r}}$  are, respectively, quantum mechanical momentum and coordinate operators. From (7) it follows that under the action of only the electric field the wavepacket will accelerate indefinitely. This never happens in metals because of scatterings on impurities, that randomly change the direction of motion. It is impossible then to trace trajectories of all wavepackets and the natural language to describe such a system is provided by the semiclassical Boltzmann equation.

In classical physics the Boltzmann equation is the evolution equation for the particle distribution in the phase space. We will always assume in this work that the system is spatially uniform on scales much larger than the distance between scatterers, where the classical Boltzmann equation for scatterings on elastic impurities has the following form [24, 25]:

$$\frac{\partial f_{\mathbf{k}}}{\partial t} - e\mathbf{E} \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}} = - \sum_{\mathbf{k}'} \omega_{\mathbf{k},\mathbf{k}'} (f_{\mathbf{k}} - f_{\mathbf{k}'}). \quad (8)$$

The rhs of (8) is called the collision term. For electrons that interact only with static impurities but not with each other the collision term is a linear functional of the distribution function. This linearity is not affected by the Pauli principle [27]. However, when many-body interactions contribute to the collision term the Pauli principle leads to contributions proportional to  $f_{\mathbf{k}}(1 - f_{\mathbf{k}'})$  etc. We will not consider the latter case in our discussion. The scattering rate  $\omega_{\mathbf{k},\mathbf{k}'}$  depends on details of the scattering potential and should be found separately. For a sufficiently smooth impurity, one can use wavepacket equations to find the scattering cross-section by purely classical means but, in most realistic applications, a smooth potential approximation does not hold for an impurity. Often the opposite limit of a  $\delta$ -function type of a potential is considered as a reasonable assumption. This fact jeopardizes the applicability of the semiclassical approach but quantum mechanics provides a simple solution. There is the *rule* that connects the quantum mechanical scattering matrix with the classical scattering rate. This rule is called the golden rule of quantum mechanics. For a weak impurity potential in the lowest Born approximation it reads [26]

$$\omega_{\mathbf{k},\mathbf{k}'} = \frac{2\pi}{\hbar} |V_{\mathbf{k},\mathbf{k}'}|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}), \quad (9)$$

where  $\epsilon_{\mathbf{k}}$  is the kinetic energy of an electron with the momentum  $\mathbf{k}$  and  $V_{\mathbf{k},\mathbf{k}'}$  is the matrix element of the disorder potential between two states of an electron before and after the scattering. In what follows we will assume that  $\hbar = 1$ . The potential of randomly placed impurities is  $V(\mathbf{r}) = \sum_i v(\mathbf{r} - \mathbf{R}_i)$ , where  $i$  enumerates impurities,  $\mathbf{R}_i$  are their

random positions and  $v(\mathbf{r} - \mathbf{R}_i)$  is the potential of the single impurity with its center placed at  $\mathbf{R}_i$ . One can show [27], that for such a disorder  $\langle |V_{\mathbf{k},\mathbf{k}'}|^2 \rangle_{\text{dis}} = n|v_{\mathbf{k}-\mathbf{k}'}|^2$ , where  $n$  is the impurity concentration and  $v_{\mathbf{q}}$  is the Fourier transform of the single impurity potential at  $\mathbf{R}_i = 0$ .

Together, the golden rule (9) and the classical Boltzmann equation (8) allow to perform the quantitative self-consistent calculation of the conductivity. Assume that the electric field is weak and look for the solution of the Boltzmann equation in the form

$$f_{\mathbf{k}} = f_{\text{eq}}(\epsilon_{\mathbf{k}}) + g_{\mathbf{k}}, \quad (10)$$

where  $f_{\text{eq}}(\epsilon_{\mathbf{k}})$  is the equilibrium distribution, which depends only on the energy of a particle and does not contribute to the current and  $g_{\mathbf{k}}$  is the correction linear in  $\mathbf{E}$ . At the steady state the term with the partial time derivative is zero and to linear order in  $\mathbf{E}$  the correction to the distribution satisfies the time independent equation

$$-e\mathbf{E} \cdot \mathbf{v}_{\mathbf{k}} \frac{\partial f_{\text{eq}}(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} = - \sum_{\mathbf{k}'} \omega_{\mathbf{k},\mathbf{k}'} (g_{\mathbf{k}} - g_{\mathbf{k}'}), \quad (11)$$

where in our case  $\mathbf{v}_{\mathbf{k}} = \mathbf{k}/m$ . Looking for the solution in the form  $g_{\mathbf{k}} = g_0 \mathbf{E} \cdot \mathbf{k}$ , one can find a self-consistent result

$$g_{\mathbf{k}} = \frac{e\tau_{\text{tr}} \mathbf{E} \cdot \mathbf{k}}{m} \cdot \frac{\partial f_{\text{eq}}(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}}, \quad (12)$$

where

$$\frac{1}{\tau_{\text{tr}}} = \sum_{\mathbf{k}'} \omega_{\mathbf{k},\mathbf{k}'} (1 - \cos(\mathbf{k}, \mathbf{k}')), \quad (13)$$

$\tau_{\text{tr}}$  is called the transport lifetime. The electric current is given by the expression

$$\mathbf{J} = -e \sum_{\mathbf{k}} g_{\mathbf{k}} \mathbf{v}_{\mathbf{k}}. \quad (14)$$

Using that at zero temperature  $\frac{\partial f_{\text{eq}}(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} = -\delta(\epsilon_{\text{F}} - \epsilon_{\mathbf{k}})$  one can arrive at the following expression for the conductivity along the electric field in the 2D electron system

$$\sigma_{xx} = \frac{e^2 k_{\text{F}} v_{\text{F}} \tau_{\text{tr}}}{4\pi m}. \quad (15)$$

The important point is that the result (15) is rigorous in the sense that when conductivity calculations are performed by formally exact quantum mechanical techniques, such as the summation of disorder averaged Feynman diagrams in the Kubo formula in the diffusive regime and disregarding higher order effects, such as the weak localization, one arrives at the same quantitative result.

### 1.2. Difficulties with the semiclassical approach in application to the AHE

The above discussion of free electrons demonstrates that it is possible to derive transport coefficients using the classical Boltzmann equation. The power of this approach is in its transparency. It operates only with concepts that have simple classical interpretations. There is no problem with the gauge invariance.

Because of its simplicity this approach is ideal for introducing to the physics of the electron transport. Many concepts of solid state physics can be explained with a sufficient rigor without using complicated Green function techniques. Also, the semiclassical approach is needed to develop the scientific intuition about the model. Having done calculations for a simple problem one can be interested in further more complicated phenomena. It is always good to have a preliminary expectation about the final result. The semiclassical approach allows to make such an incite, while it is considerably harder with other techniques.

Certainly, the semiclassical approach has limitations but it should not be considered as valid only in the classical limit. It makes rigorous estimates even for impurities that have no analog in classical physics, such as for delta-function potentials. Hence, its domain of validity is larger. However, in applications to the AHE, the semiclassical theory faced with a number of complications. Sometimes it has been speculated that the AHE is a purely quantum mechanical phenomenon that cannot be explained by classical means [28]. We will discuss later that it is not true but first, I explain the main arguments that created this skepticism.

In real crystals electrons are not free particles. They interact strongly with the periodic potential of the lattice. It has been well known that the lattice periodicity does not result in random scatterings. The Bloch theorem guarantees that eigenstates of the electron Hamiltonian in a perfect crystal have the form

$$\psi_{n\mathbf{k}}(\mathbf{r}, t) = \frac{1}{L^{D/2}} e^{i\mathbf{k} \cdot \mathbf{r} - i\epsilon_{\mathbf{k}} t} u_{n\mathbf{k}}(\mathbf{r}), \quad (16)$$

where  $u_{n\mathbf{k}}(\mathbf{r})$  is a periodic in the elementary unit cell function. Due to this simplification, one can describe other interactions, such as scatterings on lattice imperfections with an effective Hamiltonian, not dealing directly with the lattice potential. The price for this is that the wavefunction has generally a nontrivial periodic part  $u_{n\mathbf{k}}(\mathbf{r})$  and the dispersion is no longer quadratic,  $\epsilon_{\mathbf{k}} \neq \mathbf{k}^2/(2m)$  (usually it is possible to approximate it near important symmetry points by a quadratic dependence with a renormalized mass). The spectrum is also not everywhere continuous and splits into bands.

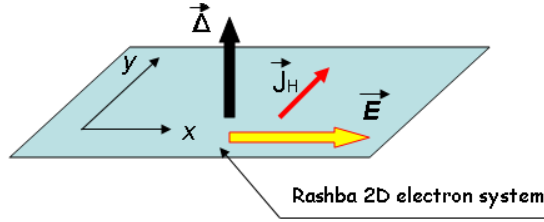
The multiple band structure plays a very important role in the theory of the AHE. Because of it, operators of many observables are matrices in the band index space, which can have nonzero off-diagonal (inter-band) elements. One of the simplest models of this kind, shown in figure 1, is the Rashba coupled 2D electron system with an additional out of plane Zeeman interaction. Its Hamiltonian reads

$$\hat{H}_0 = \frac{k^2}{2m} + \lambda(k_y \hat{\sigma}_x - k_x \hat{\sigma}_y) - \Delta \hat{\sigma}_z, \quad (17)$$

where  $\hat{\sigma}_i$  are Pauli operators. This Hamiltonian describes two bands with different dispersions

$$\epsilon^{\pm} = \frac{k^2}{2m} \mp \sqrt{(\lambda k)^2 + \Delta^2}, \quad (18)$$

where  $\pm$  stands for major/minor band indexes. The velocity



**Figure 1.** The 2D electron system described by the Hamiltonian (17). (This figure is in colour only in the electronic version)

operator  $\hat{v} = \partial \hat{H}_0 / \partial \mathbf{k}$  has the following components:

$$\begin{aligned} \hat{v}_x &= \begin{pmatrix} k_x/m & i\lambda \\ -i\lambda & k_x/m \end{pmatrix}, \\ \hat{v}_y &= \begin{pmatrix} k_y/m & \lambda \\ \lambda & k_y/m \end{pmatrix}. \end{aligned} \quad (19)$$

It is straightforward to check that neither  $\hat{v}_x$  nor  $\hat{v}_y$  commute with the Hamiltonian. This means that in the Bloch basis of eigenstates of the Hamiltonian (17), the velocity operator still has nonzero off-diagonal elements, for example,

$$\hat{v}_x = \begin{pmatrix} v_x^{++} & v_x^{+-} \\ v_x^{-+} & v_x^{--} \end{pmatrix}, \quad v_x^{+-} \neq 0, \quad v_x^{-+} \neq 0. \quad (20)$$

The semiclassical interpretation of diagonal (intra-band) matrix elements of the velocity operator is trivial. If one prepares a wavepacket made of Bloch states of one band, the free motion of such a wavepacket will be the corresponding diagonal velocity. The off-diagonal velocity matrix elements are more subtle. They do not affect the motion of a free wavepacket. Only if a coherence among states of different bands is introduced due to some perturbation can their expectation values become nonzero. This mixing can be produced e.g. by an applied external electric field. Due to the Bloch vector dependence of the periodic part of the Bloch wave, the coordinate operator generally has nonzero inter-band matrix elements

$$\langle u_{n\mathbf{k}} | \hat{\mathbf{r}} | u_{\bar{n}\mathbf{k}} \rangle = \left\langle u_{n\mathbf{k}} \left| i \frac{\partial u_{\bar{n}\mathbf{k}}}{\partial \mathbf{k}} \right. \right\rangle \neq 0, \quad (21)$$

where  $n \neq \bar{n}$  and  $\langle u_{n\mathbf{k}} | u_{\bar{n}\mathbf{k}} \rangle$  is understood as the integral of the product of periodic parts of Bloch states over the unit cell or, in the case of the Rashba Hamiltonian (17), it means the scalar product of spinor parts of Hamiltonian eigenstates.

When the electric field is applied, the total Hamiltonian has a contribution  $\hat{H}_E = e\mathbf{E} \cdot \hat{\mathbf{r}}$ , that not only accelerates wavepackets, but also mixes states of different bands. Because of this, the expectation of inter-band parts of velocity operator components becomes nonzero. In turn, this means that in the applied electric field the instantaneous velocity of the wavepacket is no longer a corresponding diagonal part of the velocity operator, but contains an extra (anomalous) component. The situation reminds the chiral anomaly in the quantum field theory [29] where the noncommutativity of the axial current operator with the Hamiltonian leads to effects, unexpected from the Hamiltonian symmetries.

Similarly to the electric field, the impurity potential also mixes states of different bands. For example, the point-like impurity potential  $V(\mathbf{r}) = V_0 \delta(\mathbf{r})$  in the chiral basis of the Rashba 2D electron gas has the following matrix form:

$$\hat{V}_{\mathbf{k},\mathbf{k}'} = \frac{V_0}{L^2} \cdot \begin{pmatrix} \langle u_{\mathbf{k}}^+ | u_{\mathbf{k}'}^+ \rangle & \langle u_{\mathbf{k}}^+ | u_{\mathbf{k}'}^- \rangle \\ \langle u_{\mathbf{k}}^- | u_{\mathbf{k}'}^+ \rangle & \langle u_{\mathbf{k}}^- | u_{\mathbf{k}'}^- \rangle \end{pmatrix}, \quad (22)$$

with nonzero off-diagonal matrix elements (see [12] for explicit expressions). This means that the impurity role does not reduce to a simple instantaneous change of a direction of the particle motion. When a wavepacket passes near such an impurity its wavefunction becomes distorted and the inter-band part of the velocity acquires a nonzero expectation due to the local band mixing. Thus in the vicinity of impurities wavepackets move along unusual trajectories.

The AHE was found to be related exactly to that type of microscopic processes. Hence the construction of the semiclassical theory of this effect faced with the problem of how to include the inter-band coherence into the purely classical description.

## 2. Early theories of the AHE

The first theoretical proposal to relate the AHE and the spin-orbit interaction was made by Karplus and Luttinger [30]. They started from the fact that due to the relativistic corrections the effective Hamiltonian of an electron in a periodic lattice potential  $V(\mathbf{r})$  has an extra contribution due to the spin-orbit interaction

$$\hat{H}_{SO} = -\frac{1}{4m^2c^2} \hat{\boldsymbol{\sigma}} \cdot (\mathbf{p} \times \nabla V). \quad (23)$$

This part of the Hamiltonian modifies Bloch wavefunctions of electrons, introducing specific Bloch vector dependence in their periodic parts  $u_{n\mathbf{k}}(\mathbf{r})$ . When the electric field is applied the corresponding term in the Hamiltonian

$$\hat{H}_E = e\mathbf{E} \cdot \hat{\mathbf{r}} \quad (24)$$

has nonzero matrix elements between states of different bands

$$\langle u_{n\mathbf{k}} | \hat{H}_E | u_{\bar{n}\mathbf{k}} \rangle = ie\mathbf{E} \cdot \left\langle u_{n\mathbf{k}} \left| \frac{\partial u_{\bar{n}\mathbf{k}}}{\partial \mathbf{k}} \right. \right\rangle \neq 0, \quad (25)$$

where  $\bar{n} \neq n$ . This band mixing ultimately leads to an unusual linear in the electric field contribution to the transverse velocity.

The spin-orbit coupling alone does not lead to the AHE because the anomalous transverse velocity, even if present, would have different signs in different degenerate bands unless the time-reversal symmetry is broken. In ferromagnets this symmetry breaking appears spontaneously due to the exchange interaction, which is often approximated in theoretical models by the mean Zeeman-like field acting on electrons spins. In the simplest picture of the AHE this Zeeman field creates a population imbalance between bands with opposite signs of the anomalous velocity thus leading to the Hall current, proportional to the magnetization. This scenario is not always correct. For example, the recent research showed that

often the strong AHE appears near points of the spectrum where the magnetization field lifts degeneracies in the band structure [19], leading to resonance features at the Fermi energies in their vicinity.

Karplus and Luttinger did not expect that their theory would be the final answer to the AHE puzzle. The reason was that the current they found was not gauge invariant, and thus could not describe the real observable. They pointed out, however, that the magnitude of the found expression and its dependence on the impurity concentration were in a good agreement with results of experimental measurements, thus suggesting that their theory captured basic microscopic physics behind the AHE and the spin-orbit coupling and the magnetization must be the forces, driving the effect.

Their theory was subsequently criticized by Smit [31, 32], who made the first effort to design the gauge invariant theory of the effect. Smit agreed with that the spin-orbit coupling is responsible for the AHE but suggested a different mechanism. His approach was semiclassical in spirit. Smit's suggestion was to look at the evolution of a wavepacket, as a semiclassical object and to design a Boltzmann-like equation to describe the evolution of the wavepacket distribution function in the phase space. Today his name is usually associated with only one of the contributions to the Hall current, called the skew scattering, which was a new effect, not discussed by Luttinger at that time. However, in addition to the idea of the skew scattering, Smit discussed other contributions. Tracing the evolution of a wavepacket he also found the anomalous velocity in the external field [32], though he did not think that this velocity contributes to the Hall conductivity because, he thought, it is exactly canceled by another effect.

Smit pointed out that the anomalous velocity follows from the change of the polarization of wavepackets by showing that the average of the coordinate of the wavepacket contains generally an additional component  $\mathbf{A}$  due to the Bloch vector dependence of the periodic part of the Bloch wavefunction

$$\mathbf{r}_c(\mathbf{k}, t) = \mathbf{v}_k t + \mathbf{A} = \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} t + \left\langle u_{\mathbf{k}} \left| i \frac{\partial}{\partial \mathbf{k}} u_{\mathbf{k}} \right. \right\rangle. \quad (26)$$

The second part  $\mathbf{A} = \langle u_{\mathbf{k}} | i \frac{\partial}{\partial \mathbf{k}} u_{\mathbf{k}} \rangle$  depends on  $\mathbf{k}$ . According to Smit, when the electric field accelerates the wavepacket, the vector  $\mathbf{k}$  changes and consequently this changes the polarization  $\mathbf{A}$ . The wavepacket becomes deformed. This evolution of the polarization leads to an additional charge transport in the transverse to the electric field direction. Smit pointed out that  $\mathbf{A}$  is not gauge invariant and rather its curl

$$\mathbf{F} = \text{curl}_{\mathbf{k}} \mathbf{A} \quad (27)$$

should enter the final result. In modern terminology  $\mathbf{A}$  and  $\mathbf{F}$  are called the Berry connection and the Berry curvature, respectively.

Smit's objection to the relevance of the anomalous velocity to the AHE conductivity also deserves a discussion. Smit pointed out that in the DC limit wavepackets cannot be constantly accelerated. While the electric field changes the polarization by accelerating wavepackets, scatterings on impurities produce on average an exactly opposite change of

$\mathbf{k}$  if the system reaches the steady state. Thus Smit concluded that coordinate shifts at scatterings should have an exactly opposite effect on the wavepackets polarization and thus on the AHE conductivity. The coordinate shifts at scatterings, first introduced by Smit [31], indeed are the important part of the modern AHE theory. They were named 'side-jumps' by Berger [33–35] who studied the effect in more detail.

Smit's work was the precursor of the modern semiclassical approach. He made the first effort to understand the anomalous Hall conductivity in classical terms such as corrections to the velocity of wavepackets, coordinate shifts at scatterings (side-jumps) and asymmetric scatterings at an impurity potential (skew scatterings). All these ideas are currently incorporated in the theory, although his conclusion about the exact cancelation of the intrinsic and the side-jump contributions is not supported by rigorous calculations.

There are two main reasons why his arguments fail. One is that the 'polarization'  $\mathbf{A}$  is not a good quantum number and, in fact, is not gauge invariant because it changes under an arbitrary momentum dependent change of the phase in the definition of Bloch states; therefore one cannot apply classical balance arguments to it. The second point, omitted by Smit, is that the side-jump can lead to the asymmetry of the distribution function even without an asymmetry in the collision term kernel in the Boltzmann equation. Such a distribution asymmetry is rather due to the change of the kinetic energy that particles experience after the side-jump in the presence of an electric field. The corresponding correction to the distribution function was named the anomalous distribution [53]. When coupled to the conventional part of the velocity  $\partial \epsilon_{\mathbf{k}} / \partial \mathbf{k}$  the anomalous distribution leads to the Hall current.

### 2.1. Luttinger's rigorous theory: the quantum Boltzmann equation

In 1958 Luttinger published a detailed study of the AHE [36] based on the rigorous quantum mechanical approach that he had designed with Kohn in a previous publication [27]. Later this approach was generalized by Lyo and Holstein to the regime of ac external fields [37]. Luttinger's theory was correct but it did not find the general acceptance as a calculation tool and later many researchers have been looking for alternative techniques. The reason was that Luttinger's approach is very nontransparent. It involves many equations that self-consistently determine nongauge-invariant values.

In this section I will try to introduce and explain Luttinger's paper. Rather than directly following his steps, the goal here is to show that it is possible to explain Luttinger's derivation with a simple schema and a different notation, according to which it is easy to classify AHE contributions in Luttinger's approach and to make connections with the semiclassical theory.

Luttinger starts with the evolution equation for the density matrix

$$\frac{\partial \hat{\rho}}{\partial t} = i[\hat{\rho}, \hat{H}], \quad (28)$$

where  $\hat{H}$  is the Hamiltonian that includes both the disorder part and the electric field

$$\hat{H} = \hat{H}_0 + V(\hat{\mathbf{r}}) + eE_x \hat{x}. \quad (29)$$

In the stationary state one should require that

$$\frac{\partial \hat{\rho}}{\partial t} = 0. \quad (30)$$

If the solution of (28) is found, the transverse electric current is given by the expression

$$J_y = -e \text{Tr}[\hat{v}_y \hat{\rho}]. \quad (31)$$

The hats mean that objects are matrices in the band index space. Since the velocity operator  $\hat{v}_y$  is diagonal in the momentum space, only the momentum-diagonal part of  $\hat{\rho}$  is needed to calculate the current. However,  $\hat{v}_y$  can have off-diagonal elements in the band index space. From (28) and (30) Luttinger derives the analog of the Boltzmann equation, which contains terms that depend only on the diagonal in the momentum space part of the density matrix. Schematically, it is useful to group terms that appear in his quantum Boltzmann equation as follows:

$$E[DT](\hat{\rho}_{\text{eq}}) - i[\hat{H}_0, \hat{\rho}_{\text{eq}}] = I_{\text{col}}(\hat{\rho}_{\text{neq}}), \quad (32)$$

where  $\hat{H}_0$  is the part of the Hamiltonian, independent of the electric field and of the disorder potential (Luttinger worked in the basis of Bloch states that diagonalize  $H_0$ ).  $\hat{\rho}_{\text{eq}}$  is the equilibrium part of the density matrix (in the presence of the disorder but in the absence of the electric field) and  $\hat{\rho}_{\text{neq}}$  is the correction, linear in  $E$ .  $[DT]$  means the ‘driving term’ which explicitly couples to the electric field. In the Bloch basis the driving term can be written as a series in powers of the disorder potential  $V$ , that starts at  $V^0$ .

$$[DT](\hat{\rho}_{\text{eq}}) = [DT]^{(0)} + V^2[DT]^{(2)} + \dots \quad (33)$$

The collision term for elastic scatterings on static impurities is linear in  $\hat{\rho}_{\text{neq}}$  and also can be written as the series that starts at  $V^2$ .

$$I_{\text{col}}(\hat{\rho}_{\text{neq}}) = V^2 I_{\text{col}}^{(2)}(\hat{\rho}_{\text{neq}}) + V^3 I_{\text{col}}^{(3)}(\hat{\rho}_{\text{neq}}) + V^4 I_{\text{col}}^{(4)}(\hat{\rho}_{\text{neq}}) + \dots \quad (34)$$

This suggests to look for the solution for the nonequilibrium part of the density matrix in the form of a series in powers of  $V$ . Separating terms of the same order in  $V$  we find the chain of equations. The first equation allows to determine the largest term in the expansion of  $\hat{\rho}_{\text{neq}}$  and others allow to express higher corrections through the lower ones. From (32) to (34) and the linearity of  $I_{\text{col}}$  as a functional of  $\hat{\rho}_{\text{neq}}$  it follows that this series begins at the term of order  $V^{-2}$ , i.e.

$$\hat{\rho}_{\text{neq}} = V^{-2} \hat{\rho}_{\text{neq}}^{(-2)} + V^{-1} \hat{\rho}_{\text{neq}}^{(-1)} + V^0 \hat{\rho}_{\text{neq}}^{(0)} + \dots \quad (35)$$

Simple power counting shows that to determine the correction of order  $V^{-2}$  it is enough to keep the driving term at

zeroth order in  $V$  and the first term in the collision part of (34), i.e.

$$E([DT]^{(0)})_{\text{diag}} = (I_{\text{col}}^{(2)}(\hat{\rho}_{\text{neq}}^{(-2)}))_{\text{diag}}, \quad (36)$$

where the index *diag* means that we take only the band-diagonal part of the expression. Luttinger found that  $\hat{\rho}_{\text{neq}}^{(-2)}$  is diagonal in the band index and does not contribute to the Hall current. It, however, makes the dominating contribution to the longitudinal current and is needed for further calculations.

Next order contribution  $\hat{\rho}_{\text{neq}}^{(-1)}$  satisfies the equation

$$I_{\text{col}}^{(2)}(\hat{\rho}_{\text{neq}}^{(-1)}) + I_{\text{col}}^{(3)}(\hat{\rho}_{\text{neq}}^{(-2)}) = 0, \quad (37)$$

where  $\hat{\rho}_{\text{neq}}^{(-2)}$  is already found by solving (36).

It turns out that  $\hat{\rho}_{\text{neq}}^{(-1)}$ , found from (37), is still diagonal in band indexes and contains the antisymmetric contribution in the transverse to the electric field direction. It leads to the transverse conductivity that, like  $\hat{\rho}_{\text{neq}}^{(-2)}$ , depends as  $1/n$  on the impurity concentration  $n$ .

At zeroth (next) order in the disorder strength, both inter-band and intra-band matrix elements become important. One can separate four distinct parts.

$$\hat{\rho}_{\text{neq}}^{(0)} = \hat{\rho}_{\text{int}} + \hat{\rho}_{sj} + \hat{\rho}_{\text{adist}} + \hat{\rho}_{sk}, \quad (38)$$

where the first two terms are purely off-diagonal and the other two are diagonal in band indexes. These contributions to the density matrix satisfy following equations.

$$E([DT]^{(0)})_{\text{off-diag}} - i[\hat{H}_0, \hat{\rho}_{\text{int}}] = 0. \quad (39)$$

Note that terms in (39) do not depend on the impurity potential.

The equation for  $\hat{\rho}_{sj}$  reads

$$-i[\hat{H}_0, \hat{\rho}_{sj}] = (I_{\text{col}}^{(2)}(\hat{\rho}_{\text{neq}}^{(-2)}))_{\text{off-diag}}. \quad (40)$$

$\hat{\rho}_{sj}$  is purely off-diagonal in band indexes and appears because the collision term  $I_{\text{col}}^{(2)}(\hat{\rho}_{\text{neq}}^{(-2)})$  has a nonzero off-diagonal part.

The next contribution is diagonal and follows from the compensation between the higher order driving term and the collision part.

$$E[DT]^{(2)} = I_{\text{col}}^{(2)}(\hat{\rho}_{\text{adist}}). \quad (41)$$

Finally, there is a contribution due to the compensation between two collision terms

$$I_{\text{col}}^{(2)}(\hat{\rho}_{sk}) + I_{\text{col}}^{(4)}(\hat{\rho}_{\text{neq}}^{(-2)}) = 0. \quad (42)$$

All four parts of the nonequilibrium density matrix in (38) contribute to the Hall current via (31). Interestingly, since they are formally of zeroth power in  $V$  and the velocity operator does not depend on  $V$  the resulting conductivity due to these contributions for a Gaussian correlated disorder becomes independent of the impurity concentration.

## 2.2. Noncommuting coordinates

Luttinger’s theory is both complete and well justified quantum mechanically. However, his approach features the same problems as other rigorous quantum mechanical techniques in applications to the AHE. It does not explain what is happening



in simple terms. What can be concluded from his work is that off-diagonal elements of the density matrix and of the velocity operator play the important role. Separately, they are not gauge invariant and only their product produced finally a gauge invariant current. Because of these complications, Luttinger did not discuss the semiclassical meaning of the derived contributions.

To resolve this issue, in 1959 Adams and Blount made an effort to create a semiclassical theory based on the introduction of noncommuting coordinates [38].

The straightforward semiclassical approach, based on preparing a wavepacket from states of the same band, may fail when the electric field is applied. Since the electric field mixes states of different bands, a part of the initially free wavepacket starts fast oscillations with frequencies  $\omega \sim \epsilon_{n,\mathbf{k}} - \epsilon_{\bar{n},\mathbf{k}}$  in comparison to the rest of it. Such a wavepacket does not satisfy the basic criteria of being a classical object because it would be composed of parts with strongly different oscillation frequencies.

The resolution of this problem was first suggested by Adams and Blount [38]. The off-diagonal part of the Hamiltonian due to the electric field can be considered as a periodic field that modifies the Bloch wavefunctions. Thus one can choose another Bloch basis, in which the term with the electric field has no inter-band matrix elements. To linear order in  $\mathbf{E} = E_x \hat{\mathbf{x}}$  the periodic part of such *modified* Bloch states reads

$$|u'_{n\mathbf{k}}\rangle = |u_{n\mathbf{k}}\rangle + ieE_x \sum_{\bar{n} \neq n} \frac{\langle u_{\bar{n}\mathbf{k}} | \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \rangle}{\epsilon_{n\mathbf{k}} - \epsilon_{\bar{n}\mathbf{k}}} |u_{\bar{n}\mathbf{k}}\rangle, \quad (43)$$

then at  $t = 0$  one can prepare a new wavepacket

$$\Psi'_{n\mathbf{k}_c}(\mathbf{r}) = \int \frac{d^D \mathbf{k}}{L^{D/2}} a(\mathbf{k}) \exp\{i(\mathbf{k} \cdot \mathbf{r})\} |u'_{n\mathbf{k}}\rangle, \quad (44)$$

which in the external electric field does not split right away into differently oscillating components. It is now instructive to calculate the velocity of the wavepacket in the transverse to the electric field direction. Let the electric field point along the  $x$ -direction and  $\hat{H} = \hat{H}_0 + eE_x \hat{x}$  is the full Hamiltonian (we do not consider impurities yet). Then the wavepacket evolves according to

$$\Psi'_{n\mathbf{k}_c}(\mathbf{r}, t) = e^{-i\hat{H}t} \Psi'_{n\mathbf{k}_c}(\mathbf{r}). \quad (45)$$

The transverse velocity is calculated as follows:

$$\begin{aligned} v_y &= \frac{d}{dt} \langle \Psi'_{n\mathbf{k}_c}(\mathbf{r}, t) | \hat{y} | \Psi'_{n\mathbf{k}_c}(\mathbf{r}, t) \rangle \\ &= \langle u'_{n\mathbf{k}} | -i \left[ \frac{\partial}{\partial k_y}, H_0 \right] | u'_{n\mathbf{k}} \rangle \\ &= \frac{\partial \epsilon_{n\mathbf{k}}}{\partial k_y} + ieE_x \left( \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \left| \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \right. \right\rangle - \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \left| \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \right. \right\rangle \right) \\ &= \frac{\partial \epsilon_{n\mathbf{k}}}{\partial k_y} - eE_x F_z^n, \end{aligned} \quad (46)$$

where  $F^n$  is called the Berry curvature of the Bloch band with index  $n$  and

$$F_z^n = \text{Im} \left( \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \left| \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \right. \right\rangle - \left\langle \frac{\partial u_{n\mathbf{k}}}{\partial k_x} \left| \frac{\partial u_{n\mathbf{k}}}{\partial k_y} \right. \right\rangle \right) \quad (47)$$

is its  $z$ -component.

The first term in the last line of (46) is just the usual velocity that equals the diagonal part of the velocity operator, while the rest of the expression is called the *anomalous velocity*. This anomalous contribution is ultimately responsible for the intrinsic AHE.

There is sometimes a misunderstanding about how the noncommuting coordinates appear in the theory. Sometimes it is simply stated that this happens to coordinate operators after the unitary transformation that switches to the basis of Bloch states. This, of course, is not true because the unitary transformation alone cannot make commuting operators noncommuting. The reason is more subtle. In the standard Bloch basis with the periodic part  $|u_{n\mathbf{k}}\rangle$  that diagonalizes  $\hat{H}_0$  the coordinate operator has the form

$$\hat{\mathbf{r}} = i \frac{\partial}{\partial \mathbf{k}} + \mathbf{A}(\mathbf{k}) + \hat{\mathbf{X}}, \quad (48)$$

where  $\mathbf{A}(\mathbf{k})$  is diagonal in band indexes and its elements are the Berry connections of Bloch bands and  $\hat{\mathbf{X}}$  is purely off-diagonal in band indexes. If we want to work with a modified Bloch band with periodic parts of Bloch states given in (43) we should switch to that new modified basis, i.e. to make the additional rotation which transforms  $|u_{n\mathbf{k}}\rangle$  into  $|u'_{n\mathbf{k}}\rangle$ . In that basis  $\hat{H}_0$  is no longer pure diagonal and contains the off-diagonal component that cancels with  $e\mathbf{E} \cdot \hat{\mathbf{X}}$ . Thus in the modified basis the full Hamiltonian has the form

$$\hat{H} = \hat{H}'_0 + e\mathbf{E} \cdot \left( i \frac{\partial}{\partial \mathbf{k}} + \mathbf{A}(\mathbf{k}) \right), \quad (49)$$

where now  $\hat{H}'_0$  is, in fact, a new operator, that has the same matrix form in the modified basis (43) as the old free Hamiltonian  $\hat{H}_0$  in the original Bloch basis  $|u_{n\mathbf{k}}\rangle$ .

In the basis (43) the Hamiltonian (49) is by construction diagonal in band indexes including terms linear in the electric field. Thus it appears to be useful to regroup the terms in the original Hamiltonian so that in the modified basis it looks like we still have the unperturbed band-diagonal part  $\hat{H}'_0$  but instead of the usual coordinate operator the electric field couples only to its projection on the subspace of a given band. The same observation holds if we consider the average of any operator over the state of the wavepacket (44), prepared from the modified Bloch states

$$\langle \Psi_{n\mathbf{k}_c}(\mathbf{r}, t) | \hat{\mathbf{r}} | \Psi_{n\mathbf{k}_c}(\mathbf{r}, t) \rangle \approx i\delta'(\mathbf{k} - \mathbf{k}_c) + \mathbf{A}_n(\mathbf{k}_c), \quad (50)$$

where we used the fact that the inter-band component of the coordinate operator has a zero expectation value and higher order terms in the electric field can be disregarded.

Summarizing, if we consider the evolution of the wavepacket made of modified Bloch states, mathematically, instead of working with band mixing by the electric field, we can assume that we still deal with the original free diagonal Hamiltonian  $\hat{H}_0$  but coordinate operators should be substituted by their projected versions

$$\hat{\mathbf{r}} \rightarrow \hat{\mathbf{r}}_c = i \frac{\partial}{\partial \mathbf{k}} + \mathbf{A}(\mathbf{k}). \quad (51)$$

The anomalous velocity appears now as the result of the noncommutativity of such modified coordinate operators. Thus for the electric field along the  $x$ -axes the transverse velocity contains a component

$$\begin{aligned} \hat{v}_y^a &= -i[\hat{y}_c, eE_x \hat{x}_c] = -ieE_x \left[ i\frac{\partial}{\partial k_y} + A_y, i\frac{\partial}{\partial k_x} + A_x \right] \\ &= -eE_x \left( \frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y} \right) = -eE_x F_z. \end{aligned} \quad (52)$$

Adams and Blount pointed that their approach can also be applied to the scattering problem on the impurity potential if the latter is sufficiently smooth so that a moving in its field wavepacket feels only a weak gradient. One can truncate the off-diagonal part of the impurity potential  $V(\hat{\mathbf{r}}) \rightarrow V(\hat{\mathbf{r}}_c)$  so that the wavepacket acquires an additional velocity

$$v_i^a = -i[\hat{r}_c^i, \hat{r}_c^j] \frac{\partial V}{\partial r_c^j}. \quad (53)$$

The comprehensive discussion of the noncommuting coordinates in Bloch bands can be found in [39]. The theory of Adams and Blount was applied by Chazalviel [40], Nozieres and Lewiner [41], Berger [33–35] and by Lyo and Holstein [42] to the AHE in III–V n-type semiconductors. Because of the degeneracy of electronic bands in their model, they had to extend the theory to the case, which today is called ‘bands with a non-Abelian Berry curvature’. They started from the standard 8-band model with a spin–orbit interaction. Due to the hybridization the conducting bands are also influenced by the spin–orbit coupling. Similarly to the above discussion, Chazalviel and Nozieres projected coordinate operators to the space of only two conducting bands. The problem, however, is that the latter have the same energy dispersions and thus the subsequent separation of conducting bands is impossible and one has to keep the off-diagonal elements of the coordinate operator in this subspace. Thus the Berry connection and the Berry curvature become  $2 \times 2$  matrices.

$$\hat{\mathbf{r}}_c = i\frac{\partial}{\partial \mathbf{k}} + \lambda \hat{\mathbf{s}} \times \mathbf{k}, \quad (54)$$

$$\mathbf{F} = 2\lambda \hat{\mathbf{s}}, \quad (55)$$

where  $\hat{\mathbf{s}}$  is the pseudospin operator acting in the space of the conducting bands index.

This non-Abelian case, however, is trivial because the Berry curvature does not depend on the Bloch vector. If one considers a 2D electron system, only the conserved out of plane component of the pseudospin enters the Hamiltonian and the problem reduces to two separate bands with the effective impurity potential

$$V(\mathbf{r}) \rightarrow V(\mathbf{r}) + \lambda \hat{\mathbf{s}} \cdot (\mathbf{k} \times \nabla V(\mathbf{r})). \quad (56)$$

The second term in (56) is functionally similar to the spin–orbit coupling due to relativistic corrections (23) but with a different strength  $\lambda$ , which can be considered as a renormalized spin–orbit coupling constant. Formally, corrections to the impurity potential and to the coordinate operator (54) and (56) should be included in the full Hamiltonian of the 2D electron

gas, together with the Rashba coupling. However, their effects are usually weak because of the weakness of the parameter  $\lambda$  in (56), that makes the corresponding Hall conductivity also small [40]. In contrast, the Hall effect due to the Rashba coupling is nonperturbative. For example, the estimates of the intrinsic contribution for the Rashba coupled electron gas show the strength close to the universal value  $e^2/2h$  in some range of parameters [5]; so the effect of the Rashba term on the AHE is expected to dominate, although at large Fermi energies there can be a crossover between effects of two types of spin–orbit couplings.

The weakness of the Hall effect due to the coupling  $\lambda$  in (56) can be understood in terms of topological defects in the band structure. Nonzero  $\lambda$  is induced by a weak mixing of p-type orbitals to states of the conducting bands; hence it is suppressed, approximately inversely proportionally to the cubic power of the large gap between conducting and valence bands [40]. In contrast, the Rashba coupling, even when small, creates the topological defect centered directly inside the conducting bands. At Fermi energies close to this ‘resonance’ point the AHE is nonperturbative in the spin–orbit coupling and hence is very strong.

Despite the partial success of Adams and Blount’s approach, their semiclassical theory has strong limitations. One is the difficulty to apply it to a short range impurity potential. Such a potential destroys the wavepacket and thus cannot be treated in a weak gradient approximation. The second problem is that this approach still operates with not strictly classical concepts such as noncommuting coordinates. This complicates the interpretation of other objects in the semiclassical theory such as the distribution function. It also complicates the derivation of the skew scattering contribution. Thus in all publications following this approach, the important part of the skew scattering contribution was missing. That part is parametrically similar to the side-jump contribution and cannot be disregarded. For example, Chazalviel’s [40] and Nozieres and Lewiner’s [41] conclusion that the total impurity concentration independent Hall conductivity in their model is the same in magnitude but has the opposite sign from the intrinsic contribution is wrong because of this omission.

### 3. The Berry phase theory of the AHE

Sundaram and Niu [43] designed a very powerful and unifying framework to study the wavepacket kinetics. Their approach is based on the derivation of the effective Lagrangian of a wavepacket moving in weak fields. The idea of the approach is that the time-dependent Schrödinger equation for a wavepacket is realized from the variational principle with the Lagrangian given by

$$L = \langle \Psi_{\mathbf{k}_c} | i\frac{d}{dt} - \hat{H} | \Psi_{\mathbf{k}_c} \rangle. \quad (57)$$

The time dependence of the wavepacket implicitly is contained in the time dependence of its average momentum  $\mathbf{k}_c$  and coordinate  $\mathbf{r}_c = \langle \Psi_{\mathbf{k}_c} | \hat{\mathbf{r}} | \Psi_{\mathbf{k}_c} \rangle$  and possibly in other explicitly time-dependent parameters in the system. This allows to

rewrite the time derivative in (57) in terms of  $\dot{\mathbf{r}}_c$  and  $\dot{\mathbf{k}}_c$

$$L = \mathbf{k}_c \dot{\mathbf{r}}_c - \epsilon(\mathbf{k}_c, \mathbf{r}_c) + \dot{\mathbf{k}}_c \left\langle u \left| \frac{\partial u}{\partial \mathbf{k}_c} \right. \right\rangle + \dot{\mathbf{r}}_c \left\langle u \left| \frac{\partial u}{\partial \mathbf{r}_c} \right. \right\rangle + \left\langle u \left| \frac{\partial u}{\partial t} \right. \right\rangle, \quad (58)$$

where  $|u\rangle$  is the unit cell periodic part of the Bloch wave.

The first two terms in the Lagrangian (58) are the same as in a typical Lagrangian of a classical particle with the classical mechanical Hamiltonian  $H_{cl} = \epsilon(\mathbf{k}_c, \mathbf{r}_c)$ . The other terms are geometric, in the sense that their contribution to the action depends on the trajectory in the phase space but not on the rate of the motion along this trajectory. This is the feature of the Berry phase in quantum mechanics and effects of the last three terms in (58) can be called Berry phase effects.

The Lagrangian formulation provides a fully gauge invariant approach to the study of the wavepacket dynamics. It is now easy to find the equations of motion in an arbitrary potential with a weak gradient in a magnetic field  $\mathbf{B}$  by varying the action over the trajectory. For the motion in a band with a dispersion  $\epsilon_{\mathbf{k}}$  the result reads

$$\begin{aligned} \dot{\mathbf{r}}_c &= \frac{\partial \epsilon_{\mathbf{k}_c}}{\partial \mathbf{k}_c} - \dot{\mathbf{k}}_c \times \mathbf{F}, \\ \dot{\mathbf{k}}_c &= -e\mathbf{E} - \nabla V(\mathbf{r}_c) - e\dot{\mathbf{r}}_c \times \mathbf{B}, \end{aligned} \quad (59)$$

where  $\mathbf{F}$  is the Berry curvature of the Bloch band. Wavepacket equations show that the Berry curvature can be considered as an unusual magnetic field acting in the momentum space. However, unlike the magnetic field in electrodynamics, which is a pure curl, the Berry curvature originates from a source. In electrodynamics, a magnetic field with such properties would originate from magnetic monopoles. Their analogs in Bloch bands are the points of exact crossings of band dispersion curves [39, 19].

The wavepacket equations can be generalized when the motion in degenerate bands is considered. If states of degenerate bands mix coherently the evolution becomes more complicated. The state of the wavepacket should then be considered having finite amplitudes in both bands [44, 45]

$$|\Psi_{\mathbf{k}_c}\rangle = \int d\mathbf{k} a(\mathbf{k}) [\eta_1 |\Psi_1\rangle + \eta_2 |\Psi_2\rangle], \quad (60)$$

where  $|\Psi_i\rangle$  ( $i = 1, 2$ ) are basis functions of the wavepackets in each band. The coefficients  $\eta_i$  enter the effective Lagrangian and should be considered as independent variables. Their dynamics was found to be according to equations

$$i \frac{d\eta_i}{dt} = \left( H_{ij} - \dot{\mathbf{k}}_c \left\langle u_i \left| i \frac{\partial u_j}{\partial \mathbf{k}_c} \right. \right\rangle \right) \eta_j, \quad (61)$$

where  $H_{ij}$  are matrix elements of the Hamiltonian.

### 3.1. The anomalous Nernst effect

The recent triumph of the wavepacket approach was the first semiclassical explanation and the quantitative theory of the intrinsic anomalous Nernst effect (ANE), which is the

AHE driven not by an external electric field but rather by the temperature gradient. The theory of the ANE [46] is based on the previous understanding of the intrinsic angular momentum [43, 47] of a wavepacket and also on the observation [48] that the wavepacket equations (59) lead to the specific expression for the phase space volume. When considering the continuous limit it reads

$$\sum_{\mathbf{k}} \rightarrow \int [d\mathbf{k}] (1 + e\mathbf{B} \cdot \mathbf{F}). \quad (62)$$

The physically measurable transport current is defined by

$$\mathbf{j} = \mathbf{J} - \nabla \times \mathbf{M}(\mathbf{r}), \quad (63)$$

where  $\mathbf{J}$  is the microscopic current and  $\mathbf{M}(\mathbf{r})$  is the magnetization density. The latter can be found from the grand canonical potential in the magnetic field

$$\begin{aligned} F &= -\frac{1}{\beta} \sum_{\mathbf{k}} \log(1 + e^{-\beta(\epsilon_M - \mu)}) \\ &= \frac{1}{\beta} \int [d\mathbf{k}] (1 + e\mathbf{B} \cdot \mathbf{F}) \log(1 + e^{-\beta(\epsilon_M - \mu)}), \end{aligned} \quad (64)$$

where  $\beta = 1/k_B T$  and  $\epsilon_M = \epsilon(\mathbf{k}) - \mathbf{m}(\mathbf{k}) \cdot \mathbf{B}$  is the electron energy in the magnetic field coupled to the magnetic moment of a wavepacket  $\mathbf{m}(\mathbf{k}) = -i(e/2) \langle \nabla_{\mathbf{k}} u | \times [\hat{H}(\mathbf{k}) - \epsilon_{\mathbf{k}}] | \nabla_{\mathbf{k}} u \rangle$ .

The magnetization is the magnetic field derivative of the thermodynamic potential

$$\mathbf{M}(\mathbf{r}) = - \left( \frac{\partial F}{\partial \mathbf{B}} \right)_{\mu, T}. \quad (65)$$

The expression for the intrinsic Hall current, induced by a weak temperature gradient originates from the phase space volume correction in (64). Substituting (65) and (64) into (63) one can find [46]

$$\begin{aligned} \mathbf{j}_{\text{int}} &= -e \frac{\nabla T}{T} \times \int [d\mathbf{k}] \mathbf{F} [(\epsilon_M - \mu) f_0(\epsilon_{\mathbf{k}}) \\ &\quad \times k_B T \log(1 + e^{-\beta(\epsilon_M - \mu)})]. \end{aligned} \quad (66)$$

### 3.2. Wavepacket theory of intrinsic contribution and the side-jump effect

The intrinsic contribution to the AHE is a straightforward consequence of the anomalous velocity term in wavepacket equations (59). Under the action of the electric field, all the electrons in the Fermi sea will shift in the transverse direction, leading to the intrinsic Hall current [1]

$$\mathbf{J}^{\text{int}} = -e^2 \mathbf{E} \times \int [d\mathbf{k}] f_{\mathbf{k}} \mathbf{F}, \quad (67)$$

where  $f_{\mathbf{k}}$  is the electron distribution function in the given band and  $\mathbf{F}$  is the Berry curvature.

Sinitzyn *et al* demonstrated [7] that wavepacket equations can also be successfully applied to the problem of a scattering on an impurity, if the latter has a sufficiently smooth potential, thus providing the fully gauge invariant theory of the side-jump effect. Integrating (59) over the time interval during which a wavepacket ‘feels’ the impurity potential and assuming that

this potential is sufficiently weak, one can find a coordinate shift at a scattering event

$$\delta \mathbf{r}_{\mathbf{k},\mathbf{k}'}^a = \mathbf{F} \times (\mathbf{k}' - \mathbf{k}), \quad (68)$$

where  $\mathbf{k}'$  and  $\mathbf{k}$  are center of mass momentums of the wavepacket, respectively, after and before the scattering. This definition of the anomalous coordinate shift at a scattering on an impurity (the side-jump) is different from some expressions suggested in early theories. For example Berger [21, 22] assumed that  $\delta y^a \sim k_x$ . Berger's definition follows from the identification of the coordinate shift with the Berry connection. Since the Berry connection is not gauge invariant, the old definition does not have a direct semiclassical meaning. In contrast, the expression (68) as well as more general expressions (74), (75) from next section are gauge invariant and depend both on the in-going  $\mathbf{k}$  and the out-going  $\mathbf{k}'$  Bloch vectors. This difference becomes important when constructing the rigorous theory of the effect when the scattering on an impurity is not isotropic.

There are two main rather distinct effects due to the anomalous shift. One is the side-jump accumulation. After averaging over many scatterings, side-jumps do not cancel and lead to the velocity renormalization by a correction

$$v_y^{(sj)}(\mathbf{k}) = \sum_{\mathbf{k}'} \omega_{\mathbf{k}',\mathbf{k}} \delta \mathbf{r}_{\mathbf{k}',\mathbf{k}}^a. \quad (69)$$

The second effect is that when a scattering takes place in the presence of an external electric field, there is a change in the potential energy upon a scattering given by

$$\Delta U_{\mathbf{k},\mathbf{k}'} = e\mathbf{E} \cdot \delta \mathbf{r}_{\mathbf{k}',\mathbf{k}}^a. \quad (70)$$

This change of energy ultimately influences the Hall conductivity and should be properly included in the semiclassical Boltzmann equation.

According to [7], the side-jump related conductivities depend only on parameters taken near the Fermi surface. This is in contrast to the intrinsic contribution that depends on the integral of the Berry curvature over the whole Fermi sea. This may be one of the reasons why the comparison with experiments showed a good agreement with the intrinsic contribution calculations that disregarded impurity effects, except keeping a finite lifetime of quasiparticles [4]. Although the intrinsic and the side-jump contributions to the transverse conductivity do not depend on impurity concentrations and in this sense are parametrically similar, still if the Berry curvature is weak near the Fermi surface but strong deep inside of it, the intrinsic contribution can dominate.

The ultimate example of this kind is the quantum anomalous Hall effect that appears when the Fermi level is placed inside the gap in the bulk spectrum. In such insulators the gapless excitations are forbidden (except near the sample edges), so the side-jump and the skew scattering effects do not contribute to the conductivity but if the band has a nonzero Berry curvature there is a quantized intrinsic contribution to the Hall current. This happens e.g. in 2D Dirac bands, related to the graphene system [49, 50].

## 4. Scattering rules

The ‘philosophy’ of the semiclassical approach is to operate only with classical concepts, however, using several rules that connect some of them with purely quantum mechanical ones in order to achieve a quantitatively rigorous result. The expression for the Berry curvature is one of such rules, namely it relates the anomalous velocity to Bloch wavefunctions. The scattering is described in quantum mechanics by the scattering matrix, which has no analog in classical physics; therefore one should use the rules that connect the scattering matrix to the classical microscopic effects.

One such scattering rule is widely known, and for its importance it is named the *golden rule* of quantum mechanics. Lets introduce a combined band–momentum index  $l = (n, \mathbf{k})$ . The golden rule relates the scattering rate  $\omega_{l'l'}$  from the state  $l'$  into the state  $l$  in the continuous spectrum with the corresponding element of the scattering  $T$ -matrix [26]:

$$\omega_{l'l'} = 2\pi |T_{l'l'}|^2 \delta(\epsilon_{l'} - \epsilon_l). \quad (71)$$

The  $T$ -matrix is defined as

$$T_{l'l'} = \langle l | \hat{V} | \psi_{l'} \rangle, \quad (72)$$

where  $\hat{V}$  is the impurity potential operator and  $|\psi_{l'}\rangle$  is the eigenstate of the full Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{V}$  that satisfies the Lippman–Schwinger equation

$$|\psi_{l'}\rangle = |l\rangle + \frac{\hat{V}}{\epsilon_l - \hat{H}_0 + i\eta} |\psi_{l'}\rangle. \quad (73)$$

Scattering rates  $\omega_{l'l'}$  cannot include all the possible information encoded in the scattering matrix. This is obvious because entries of the  $T$ -matrix are complex numbers and entries of the matrix of scattering rates are real. In the golden rule only the absolute value of the  $T$ -matrix elements are represented. Thus the semiclassical approach, which uses only the golden rule as relating the classical and the quantum descriptions of the scattering, should generally fail. This is indeed the case in the AHE. The golden rule does not contain the information about the side-jump effect at a scattering event. This fact forced authors of [51] to search for the gauge invariant expression for the side jump that would connect it to the scattering matrix.

Such an expression indeed can be derived. In the lowest Born approximation it has a particularly simple form,

$$\delta \mathbf{r}_{l'l} = \left\langle u_{l'} \left| i \frac{\partial}{\partial \mathbf{k}'} u_{l'} \right. \right\rangle - \left\langle u_l \left| i \frac{\partial}{\partial \mathbf{k}} u_l \right. \right\rangle - \hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}} \arg(V_{l',l}), \quad (74)$$

where  $\arg[a]$  is the phase of the complex number  $a$  and

$$\hat{\mathbf{D}}_{\mathbf{k}',\mathbf{k}} = \frac{\partial}{\partial \mathbf{k}'} + \frac{\partial}{\partial \mathbf{k}}.$$

This type of expression has been first found even before the work [51], however, beyond the AHE theory. Belinicher *et al* derived it to apply in the photovoltaic effect [52]. They showed that when electrons absorb a polarized light they make shifts (74), where  $V$  would be responsible for the

electron–photon interaction. Such shifts of the form (74) finally contributed to the photo-induced conductivity in their model. Unfortunately the work [52] had been unnoticed by the modern Hall effect community until the expression (74) was independently rederived in [51] and applied to the AHE problem.

The expression for the side jump (74) is gauge invariant. Interestingly, it restores the information, lost in the golden rule. Unlike the golden rule that in the lowest Born approximation depends on the absolute value of the scattering potential, the coordinate shift expression depends on its phase but does not depend on its absolute value. Thus the expression (74) can be considered as complimentary to the golden rule.

If the impurity potential is spin independent, then the side-jump does not depend explicitly on the type of the impurity potential and can be expressed in terms of initial and final states only [51, 53]:

$$\delta \mathbf{r}_{l'l} = \left\langle u_{l'} \left| i \frac{\partial}{\partial \mathbf{k}'} u_{l'} \right. \right\rangle - \left\langle u_l \left| i \frac{\partial}{\partial \mathbf{k}} u_l \right. \right\rangle - \hat{\mathbf{D}}_{\mathbf{k}', \mathbf{k}} \arg[\langle u_{l'} | u_l \rangle]. \quad (75)$$

At a weak scattering angle it reduces to equation (68), derived in the previous section [49]. The derivation of the golden rule (71) and the expression for the coordinate shift (75) can be done by considering a scattering of a wavepacket. Imagine a state, that initially coincides with the Bloch state  $\psi_l(\mathbf{r}, t)$  under the influence of a weak potential of an impurity  $V(\mathbf{r})$ . The solution of the time-dependent Schrödinger equation can be written in terms of the eigenvectors  $\psi_{l'}(\mathbf{r}, t)$  of the unperturbed Hamiltonian

$$\psi_l^{\text{out}}(\mathbf{r}, t) = \sum_{l'} C_{l'}(t) \psi_{l'}(\mathbf{r}, t). \quad (76)$$

Consider the wavepacket, that was initially gathered around the state  $l$ . Then in the lowest order in the strength of the potential the perturbation theory leads to the following expression for time-dependent coefficients  $C_{l'}(t)$  (see equation 19.9 in [54]):

$$C_{l'}(t) = -iV_{l'l} \int_{-\infty}^t e^{i(\epsilon_{l'} - \epsilon_l)t'} dt' + \delta_{l'l}. \quad (77)$$

The higher order terms can be incorporated into the above formula by merely substituting the  $T$ -matrix instead of the disorder matrix elements (see equation 19.10 in [54]).

$$C_{l'}(t) = -iT_{l'l} \int_{-\infty}^t e^{i(\epsilon_{l'} - \epsilon_l)t'} dt' + \delta_{l'l}. \quad (78)$$

From this solution one can show that for  $l' \neq l$ ,  $C_{l'}(t)$  change with time according to the law

$$\frac{d|C_{l'}(t)|^2}{dt} = 2\pi |T_{l'l}|^2 \delta(\epsilon_{l'} - \epsilon_l). \quad (79)$$

The coefficient  $|C_{l'}(t)|^2$  has the meaning of the probability of the electron to be in the state  $l'$ , from which immediately the golden rule (71) follows.

The coordinate shift expression was derived in a similar fashion. One can prepare a wavepacket, approaching the impurity at the point  $\mathbf{r}_{\text{imp}} = 0$  according to the law  $\mathbf{r}(t) = \mathbf{v}_0 t$

at  $t \rightarrow -\infty$ . The scattering on an impurity generally destroys the wavepacket, however having the scattering matrix one can write a formal expression for the average coordinate of the state of the wavepacket after the scattering. According to [51] it can be written in the form

$$\begin{aligned} \mathbf{r}_{+\infty} &= \int d\mathbf{r} (\Psi^{\text{out}}(\mathbf{r}, +\infty))^* \mathbf{r} \Psi^{\text{out}}(\mathbf{r}, +\infty) \\ &= \sum_{l'} |C_{l'}(t \rightarrow +\infty)|^2 (\mathbf{v}_0 t + \delta \mathbf{r}_{l'l}). \end{aligned} \quad (80)$$

Since  $|C_{l'}(t \rightarrow +\infty)|^2$  has the classical meaning of the scattering probability into the state  $l'$ , the expression in the parentheses is reasonable to interpret as the coordinate of the particle if it is scattered in the state  $l'$ . Then the term  $\mathbf{v}_0 t$  simply tells that after the scattering the particle moves with the new velocity  $\mathbf{v}_0$  and thus the expression  $\delta \mathbf{r}_{l'l}$  in (80) can be interpreted as the coordinate shift at a scattering event. This identification leads finally to the gauge invariant expression (74).

The side-jump is a weak effect and thus its expression in the lowest Born approximation is sufficient for further discussion. However the lowest Born approximation in the golden rule is inappropriate for the theory of the AHE. For a weak disorder one can use the expression of the  $T$ -matrix in terms of the Born series in powers of disorder potential matrix elements

$$T_{ll'} \approx V_{ll'} + \sum_{l''} \frac{V_{ll''} V_{l''l'}}{\epsilon_l - \epsilon_{l''} + i\eta} + \dots \quad (81)$$

One can consider only several first terms in this series in order to capture the basic microscopic processes. Substituting equation (81) into (71) one will arrive at the expansion

$$\omega_{ll'} = \omega_{ll'}^{(2)} + \omega_{ll'}^{(3)} + \omega_{ll'}^{(4)} + \dots, \quad (82)$$

where

$$\omega_{ll'}^{(2)} = 2\pi \langle |V_{ll'}|^2 \rangle_{\text{dis}} \delta(\epsilon_l - \epsilon_{l'}), \quad (83)$$

$$\omega_{ll'}^{(3)} = 2\pi \left( \sum_{l''} \frac{\langle V_{ll''} V_{l''l'} V_{l'l} \rangle_{\text{dis}}}{\epsilon_l - \epsilon_{l''} - i\eta} + \text{c.c.} \right) \delta(\epsilon_l - \epsilon_{l'}), \quad (84)$$

and so on. The skew scattering contribution to the Hall effect follows from the antisymmetric part of the scattering rate

$$\omega_{ll'}^{(a)} \equiv \frac{\omega_{ll'} - \omega_{l'l}}{2}. \quad (85)$$

Since  $\omega_{ll'}^{(2)}$  is symmetric, the leading contribution to  $\omega_{ll'}^{(a)}$  appears at order  $V^3$ , at which the antisymmetric part of the scattering rate is particularly simple [36, 55]

$$\begin{aligned} \omega_{ll'}^{(3a)} &= -(2\pi)^2 \sum_{l''} \delta(\epsilon_l - \epsilon_{l''}) \text{Im} \langle V_{ll''} V_{l''l'} V_{l'l} \rangle_{\text{dis}} \\ &\times \delta(\epsilon_l - \epsilon_{l'}), \end{aligned} \quad (86)$$

with the superscript  $3a$  meaning that this is the antisymmetric part of the scattering rate calculated at order  $V^3$ . Usually, properties of the skew scattering were inferred only from this lowest order antisymmetric part of  $\omega_{ll'}$ . Thus it is customarily assumed that  $\omega_{ll'}^{(a)}$  is proportional to the impurity concentration. This, however, holds only in the lowest nonzero order, i.e. for

$\omega_{ll'}^{(3a)}$ . In the next order the antisymmetric scattering is proportional to the product of four disorder vertexes. For a Gaussian correlated potential  $\langle V \cdot V \cdot V \cdot V \rangle_{\text{dis}} \sim \langle V \cdot V \rangle_{\text{dis}} \langle V \cdot V \rangle_{\text{dis}} \sim n^2$ , where  $n$  is the impurity concentration. Thus the higher order contribution behaves as  $\omega_{ll'}^{(4a)} \sim n^2$ , unlike  $\omega_{ll'}^{(3a)} \sim n$ . This means that the higher order term is different parametrically and has a rather distinct microscopic origin; therefore it should not be disregarded. Moreover, the contribution to the conductivity, arising from  $\omega_{ll'}^{(4a)}$ , is parametrically similar to the side-jump related contributions. Hence, to derive all important effects one should calculate the symmetric part of  $\omega_{ll'}$  in the lowest Born approximation and then calculate its antisymmetric part, including the next *two* orders in  $V$ .

$$\omega_{ll'} \approx \omega_{ll'}^{(2)} + \omega_{ll'}^{(3a)} + \omega_{ll'}^{(4a)}. \quad (87)$$

### 5. Mechanisms of the AHE in the semiclassical Boltzmann equation

Equations (71) and (75) contain the quantum mechanical information necessary to achieve quantitatively rigorous predictions working in the framework of the semiclassical Boltzmann equation. This approach takes into account both the change of the direction and the coordinate shift during a scattering in a homogeneous crystal in the presence of a driving electric field  $\mathbf{E}$ . Keeping only terms up to the linear order in the electric field the Boltzmann equation reads [53]

$$\begin{aligned} \frac{\partial f_l}{\partial t} - e\mathbf{E} \cdot \mathbf{v}_{0l} \frac{\partial f_0(\epsilon_l)}{\partial \epsilon_l} \\ = \sum_{l'} \omega_{ll'} \left[ f_l - f_{l'} - \frac{\partial f_0(\epsilon_l)}{\partial \epsilon_l} e\mathbf{E} \cdot \delta \mathbf{r}_{ll'} \right], \end{aligned} \quad (88)$$

where expressions for  $\omega_{ll'}$  and  $\delta \mathbf{r}_{ll'}$  were derived in the previous section,  $\mathbf{v}_{0l}$  is the usual velocity

$$\mathbf{v}_{0l} = \partial \epsilon_l / \partial \mathbf{k} \quad (89)$$

and  $f_0(\epsilon_l)$  is the equilibrium distribution.

The Boltzmann-type equation (88) has the standard form, as (8) for free electrons, except the allowed inter-band transitions and the coordinate shift effect which is taken into account in the last term in the collision integral on the rhs of equation (88). The derivation of this term has been explained in [7, 49, 53]. It follows from the fact that under the scattering in the electric field from the state  $l'$  into the state  $l$ , the side-jump is associated with the change of the potential energy  $\Delta U_{ll'} = e\mathbf{E} \cdot \delta \mathbf{r}_{ll'}$ , which has to be compensated by the change of the kinetic energy. Thus the conservation of energy requires that  $\epsilon_{l'} - \epsilon_l = e\mathbf{E} \cdot \delta \mathbf{r}_{ll'}$ . This in turn means that the equilibrium distribution does not annihilate the collision term anymore because  $f_0(\epsilon_l) - f_0(\epsilon_{l'}) \approx -\frac{\partial f_0(\epsilon_l)}{\partial \epsilon_l} e\mathbf{E} \cdot \delta \mathbf{r}_{ll'}$ , which is exactly the last term in (88). The validity of these arguments was confirmed in numerical simulations [7].

The total distribution function  $f_l$  in the steady state ( $\partial f_l / \partial t = 0$ ) can be written as

$$f_l = f_0(\epsilon_l) + g_l^s + g_l^{a1} + g_l^{a2} + g_l^{\text{adist}}, \quad (90)$$

where  $g_l^s$ ,  $g_l^{a1}$ ,  $g_l^{a2}$  and  $g_l^{\text{adist}}$  are nonequilibrium corrections to the distribution function of linear order in the electric field (the label adist stands for the anomalous distribution). They solve self-consistent time-independent equations [53]

$$-e\mathbf{E} \cdot \mathbf{v}_{0l} \frac{\partial f_0(\epsilon_l)}{\partial \epsilon_l} = -\sum_{l'} \omega_{ll'}^{(2)} (g_l^s - g_{l'}^s), \quad (91)$$

$$\sum_{l'} \omega_{ll'}^{(3a)} (g_l^s - g_{l'}^s) + \sum_{l'} \omega_{ll'}^{(2)} (g_l^{a1} - g_{l'}^{a1}) = 0, \quad (92)$$

$$\sum_{l'} \omega_{ll'}^{(4a)} (g_l^s - g_{l'}^s) + \sum_{l'} \omega_{ll'}^{(2)} (g_l^{a2} - g_{l'}^{a2}) = 0 \quad (93)$$

and

$$\sum_{l'} \omega_{ll'} \left( g_l^{\text{adist}} - g_{l'}^{\text{adist}} - \frac{\partial f_0(\epsilon_l)}{\partial \epsilon_l} e\mathbf{E} \cdot \delta \mathbf{r}_{ll'} \right) = 0. \quad (94)$$

One can deduce the dependence of the distribution corrections on the impurity concentration by noticing that  $\omega_{ll'}^{(2)} \sim n$ , then from (91) follows that  $g_l^s \sim n^{-1}$ . Then from (92) and the fact that  $\omega_{ll'}^{(3a)} \sim n$  follows that  $g_l^{a1} \sim n^{-1}$ , then from  $\omega_{ll'}^{(4a)} \sim n^2$  and (93) follows that  $g_l^{a2} \sim n^0$  and from (94) follows  $g_l^{\text{adist}} \sim n^0$ . A detailed solution of equations (91)–(94) in a special model was demonstrated in [53].

The first correction  $g_l^s$  is symmetric and others  $g_l^{\text{adist}}$ ,  $g_l^{a1}$  and  $g_l^{a2}$  are asymmetric in the transverse to the electric field direction. When coupled to the usual part of the velocity the latter lead to three separate gauge invariant contributions to the conductivity. For the electric field along the  $x$ -axes these read

$$\sigma_{yx}^{\text{adist}} = -e \sum_l (g_l^{\text{adist}} / E_x) (v_{0l})_y \sim n^0, \quad (95)$$

$$\sigma_{yx}^{\text{sk1}} = -e \sum_l (g_l^{a1} / E_x) (v_{0l})_y \sim n^{-1}, \quad (96)$$

$$\sigma_{yx}^{\text{sk2}} = -e \sum_l (g_l^{a2} / E_x) (v_{0l})_y \sim n^0. \quad (97)$$

The last two contributions can be called the skew scattering conductivities because they originate from the asymmetric part of the collision term kernel  $\omega_{ll'}$ . It is, however, reasonable to distinguish between the two because of their different dependence on the impurity concentration. The first skew scattering conductivity (96) is the *conventional skew scattering*, that has been discussed by many authors [36, 55]. The second one (97) was generally discarded, although it is parametrically the same as the side-jump conductivity. The explicit quantitative estimates of  $\sigma_{yx}^{\text{sk2}}$  so far exist only for the massive 2D Dirac band [53]. Because of the lack of the proper terminology we will call (97) the *intrinsic skew scattering* because this conductivity, similarly to the intrinsic contribution, is independent of the impurity concentration  $n$ .

The asymmetric corrections to the distribution do not exhaust all mechanisms of the AHE. We already discussed that between scatterings under the action of the electric field, wavepackets move with an extra velocity

$$\mathbf{v}_l^a = e\mathbf{E} \times \mathbf{F}_l. \quad (98)$$

**Table 1.** Mechanisms of the AHE in the semiclassical Boltzmann equation (SBE), the Luttinger quantum Boltzmann equation (QBE) and the Kubo–Streda [60] formula (KSF).  $\hat{v}_{x/y}^d$  and  $\hat{v}_{x/y}^{od}$  stand for diagonal and off-diagonal parts of the velocity operator in the Bloch state basis,  $n$  is the impurity concentration,  $\text{Tr}$  is the summation over all states in the momentum space and over all band indexes,  $G^R$ ,  $G^A$  are, respectively, retarded and advanced Green functions of the electron system and other symbols have the same meaning as in the bulk of the text.

Mechanism of the AHE	Strength of $\sigma_{yx}$	SBE $E_x \sigma_{yx}$	QBE $E_x \sigma_{yx}$	KSF $\sigma_{yx}$
Intrinsic	$O(n^0)$	$-e \text{Tr}(f_0 v_y^a)$	$-e \text{Tr}(\hat{\rho}_{\text{int}} \hat{v}_y^{\text{od}})$	$\sigma_{yx}^{\text{II}} + \sigma_{yx}^{\text{I,int}}$
Side-jump accumulation	$O(n^0)$	$-e \text{Tr}(g^s v_y^{sj})$	$-e \text{Tr}(\hat{\rho}_{sj} \hat{v}_y^{\text{od}})$	$\frac{e^2}{2\pi} \text{Tr}(\hat{v}_y^{\text{od}} \hat{G}^R \hat{v}_x^d \hat{G}^A)$
Anomalous distribution	$O(n^0)$	$-e \text{Tr}(g^{\text{adist}} v_{0y})$	$-e \text{Tr}(\hat{\rho}_{\text{adist}} \hat{v}_y^d)$	$\frac{e^2}{2\pi} \text{Tr}(\hat{v}_y^d \hat{G}^R \hat{v}_x^{\text{od}} \hat{G}^A)$
Conventional skew scattering	$O(n^{-1})$	$-e \text{Tr}(g^{a1} v_{0y})$ ( $\omega_{\mathbf{k},\mathbf{k}'}^a \sim n$ )	$-e \text{Tr}(\hat{\rho}^{(-1)} \hat{v}_y^d)$	$\frac{e^2}{2\pi} \text{Tr}(\hat{v}_y^d \hat{G}^R \hat{v}_x^d \hat{G}^A)$ (non-Gaussian vertex)
Intrinsic skew scattering	$O(n^0)$	$-e \text{Tr}(g^{a2} v_{0y})$ ( $\omega_{\mathbf{k},\mathbf{k}'}^a \sim n^2$ )	$-e \text{Tr}(\hat{\rho}_{sk} \hat{v}_y^d)$	$\frac{e^2}{2\pi} \text{Tr}(\hat{v}_y^d \hat{G}^R \hat{v}_x^d \hat{G}^A)$ (Gaussian vertex)

This velocity is linear in the electric field, therefore we did not consider its effect on the distribution function. However, when coupled to the equilibrium part of the distribution it produces a finite Hall current.

$$\sigma_{yx}^{\text{int}} = e^2 \sum_l f_0(\epsilon_l) F_l \sim n^0. \quad (99)$$

Finally, the accumulation of coordinate shifts after many scatterings can be described semiclassically on average as an additional velocity contribution

$$\mathbf{v}_l^{sj} = \sum_{l'} \omega_{l'l} \delta \mathbf{r}_{l'l}, \quad (100)$$

$$\sigma_{yx}^{sj} = -e \sum_l (g_l^s / E_x) \left( \sum_{l'} \omega_{l'l} (\delta \mathbf{r}_{l'l})_y \right) \sim n^0. \quad (101)$$

Thus the total transverse conductivity can be written as the sum of five contributions:

$$\sigma_{yx}^{\text{total}} = \sigma_{yx}^{\text{int}} + \sigma_{yx}^{\text{adist}} + \sigma_{yx}^{sj} + \sigma_{yx}^{sk1} + \sigma_{yx}^{sk2}. \quad (102)$$

### 5.1. Semiclassical versus fully quantum mechanical techniques

Besides the semiclassical theories, the research on diluted magnetic semiconductors also stimulated theoretical interest in other quantitative approaches. Due to the relative simplicity of several important models, such as the Rashba coupled 2D electron system, a number of publications appeared recently with rigorous quantum mechanical calculations by Kubo and Kubo–Streda formulas [6, 10, 13, 49, 53, 56, 57] and by a variety of the quantum Boltzmann equation and the Keldysh techniques [8, 9, 58, 59]. Sinitsyn *et al* [51, 53] demonstrated the 1–1 correspondence between semiclassical contributions to the AHE and the summation of relevant subseries of Feynman diagrams in the Kubo–Streda formula [60]. Similar agreement was established with Luttinger’s theory [36]. The results are summarized in table 1.

According to [53], the classification of contributions in the Kubo formula is not merely by a separation of diagrams into the disorder free part and the vertex correction but rather by the parts of the velocity matrices in chiral basis that stay inside the trace of the Kubo formula. Thus the intrinsic contribution appears from the summation of all diagrams with only off-diagonal parts of the velocity vertexes in Bloch basis. From this point of view the skew scattering is the most ‘classical’ because it is due to the summation of all diagrams with only diagonal parts of velocity operators and the difference between conventional and intrinsic skew scatterings is due to different types of disorder vertexes involved. The conventional skew scattering is due to the vertex correction that involved correlators of three or more disorder vertexes while the intrinsic skew scattering is due to only Gaussian disorder correlations. The side-jump and the anomalous distribution effects are related to Feynman diagrams that contain one off-diagonal (inter-band) and one diagonal (intra-band) parts of the velocity operator. This reflects the fact that although the side-jump itself is related to the anomalous velocity it contributes to the final current only after the electric field distorts the distribution function by a simple acceleration, i.e. by the coupling to the usual velocity in the Boltzmann equation or coordinate shifts create an anomalous distribution that again contributes to the final current via the coupling to the usual velocity.

### 5.2. Terminology in the AHE theory

After the above discussion of all the effects leading to the AHE it seems appropriate to reconcile some of the differences in the terminology in recent publications. Generally it is stated that there are three basic microscopic effects, leading to the Hall current: the intrinsic contribution, the side-jump and the skew scattering. Table 1 shows that this classification is too restrictive. There are, in fact, five separate gauge invariant contributions, each having rather distinct origins. It is possible to regroup them into three, because the side-jump accumulation and the anomalous distribution both originate

from coordinate shifts at scattering events; similarly, the conventional and the intrinsic skew scatterings both appear from the asymmetry in the collision term kernel in the semiclassical Boltzmann equation.

However, such a simplified classification into only three parts was one of the reasons for confusion. For example, it is customarily stated that the skew scattering always leads to the conductivity that depends as  $1/n$  on the impurity concentration. Table 1 shows that this is not true. The intrinsic skew scattering conductivity is independent of the impurity concentration and is parametrically very similar to the side-jump related contributions. Unjustified claims resulted in the omission of the intrinsic skew scattering in almost all discussions of the semiclassical approach to the AHE. Such an omission has been repeated in the recent efforts to design the spin Hall effect theory by the analogy with previous AHE results [22]. It is also useful to distinguish the side-jump accumulation and the anomalous distribution effects. The side-jump accumulation is a rather direct consequence of coordinate shifts while the derivation of the anomalous distribution requires several extra steps in the semiclassical theory, which were unnoticed in a few former publications.

Another confusing example from the recent terminology is the statement that the vertex correction, coming from a Gaussian correlated disorder in the Kubo formula is due to the side-jump effect only. Comparing the vertex correction with the semiclassical expression for the side-jump conductivity, discussed by Berger, Nozieres and others, one would find a discrepancy because the intrinsic skew scattering is also captured by the vertex correction and it was not considered by the older semiclassical theories that concentrated only on the side-jump effect.

The classification into the ‘intrinsic’ and ‘extrinsic’ contributions was also understood quite arbitrarily by many authors. In the present review we coined the word ‘intrinsic’ for the single special contribution, which is due to unusual trajectories of wavepackets in the external electric field rather than any other mechanism that involves scatterings on impurities. This definition of the intrinsic contribution is justified by the fact that it follows only from the crystal band structure. Respectively, all other contributions can be called extrinsic. Sometimes, in other publications [19] any conductivity contribution, independent of the impurity concentration  $n$  is called intrinsic. This seems not a good choice of terminology because the side-jump and the intrinsic skew scattering effects satisfy this definition but originate from scatterings on impurities. While corresponding conductivities are independent of  $n$  they can depend on other disorder parameters, for example, impurities with different typical ranges of scattering angles can result in Hall conductivities different by a numerical factor of order unity.

There are examples where the ‘intrinsic’ is associated with any effect induced by the Berry curvature in Bloch bands, while ‘extrinsic’ would be due to relativistic corrections to the impurity potential, possibly renormalized in conducting bands by the crystal potential, as discussed by Berger, Chazalviel and others [33, 40, 41]. For example, according to this terminology all effects produced in the 2D electron system by the Rashba

spin–orbit coupling are intrinsic and all other effects such as due to the spin–orbit part of the impurity potential are extrinsic. In such a case all the effects discussed in this review would be called intrinsic. Such terminology also seems somewhat misleading, because effects due to the disorder spin–orbit coupling also can be described and classified in the same way as here when working with the relativistic Dirac equation for electrons or, in the case of semiconductors, this corresponds to working with the 8-band model without projecting all operators to the conducting 2-band system. Then one can work with a disorder potential free of the spin–orbit coupling and contributions to the AHE then can be derived in the same way as in this review [40, 57].

Finally, there is a notion of the ‘Berry phase’ contribution to the AHE [1]. Often it is identified with the intrinsic contribution as defined in this review. However, origins of all disorder related effects can also be traced to the Berry phase or to a nontrivial topology of Bloch bands. For example, the side-jump expression and the antisymmetric part of the scattering rate can be expressed via a topological Pancharatnam phase [51]. Therefore it is possible to speak about the Berry phase *mechanism* of the AHE, which includes all the physics discussed here but to apply this terminology to a particular contribution can be misleading.

## 6. Summary

The modern semiclassical theory rigorously takes into account all known important contributions in the model of electrons in Bloch bands interacting with static impurities. Predictions of this theory were verified with rigorous quantum mechanical techniques. However, so far the semiclassical theory of the AHE was built to deal with electrons that do not interact with each other.

The state of the art is currently at the stage similar to where the theory of electrons in metals was before Landau introduced the Fermi liquid hypothesis. The Fermi liquid theory was originally semiclassical and allowed to derive many important properties of the electron state prior to systematic diagrammatic calculations.

The important problem now is the effect of the nonzero Berry curvature on many-body interactions and only recently new publications appeared that addressed it. Thus, Haldane [61] proposed that the Berry phase can be considered as the property of quasiparticles living near the Fermi surface. In [62] Shi *et al* showed the robustness of several results of the wavepacket theory against  $e$ – $e$  interactions. Shindou and Balents in [63] studied the problem in more detail by deriving the quantum kinetic equation. The interesting finding was that the Berry curvature now acts as a pseudo-magnetic field in the extended  $(\mathbf{k}, \omega)$  space. Also, Shi and Niu [64] considered interacting wavepackets in bands with the Berry curvature and found the attracting force that can induce the instability in the p-channel and thus can facilitate the unconventional superconductivity. More generally, there is a strong similarity between properties of systems with the AHE and the p-type superconductivity and superfluidity in  $^3\text{He-A}$  [65–69]. The effective action governing low-energy physics of the  $p_x + ip_y$



superfluid contains a topological contribution, leading to the Hall effect, similar to the intrinsic contribution to the AHE in metals. It should be interesting to explore the diffusion equation for Bogoliubov's quasiparticles on this background. For example, one can expect to find effects similar to the side-jump and the skew scattering.

Another poorly understood problem is the physics near the edges in systems with the AHE. It is possible that the side-jump type scatterings from the edge lead to the edge current. Analogous phenomena are known in geometrical optics where the reflected beam is shifted from the incident point on the mirror [70–75]. This physics can be more complicated because a reflection of the beam generally changes its intrinsic angular momentum.

Recently the optically induced AHE attracted some interest both theoretically [12, 76, 77] and experimentally [78, 79]. The conventional AHE needs a magnetization in order to break the time-reversal symmetry. This requirement can be avoided if other interactions, such as with a polarized light are introduced. An observation of such an optically induced Hall current would allow exploration of the physics discussed above, avoiding many difficulties in the interpretation of the standard AHE because currently ferromagnetic samples are very dirty. So far experimental results on this topic are controversial: one group reported the observation of the effect [78] and another reported that the effect was *not* observed in GaAs at least up to the measurement uncertainty [79] with results in agreement with the classical Hanle effect. The rigorous theory of the optically induced AHE is also missing, although the semiclassical theory allows an insight to be made. For example, one can expect to find an intrinsic-like contribution due to distorted trajectories of electrons in simultaneously applied DC and circularly polarized AC electric fields. The absorption of a photon from a polarized light can induce side-jump-like shifts etc.

One more recent experiment demonstrated that the anomalous Hall conductivity can be measurable even in paramagnetic materials when electron spins are polarized by an applied external magnetic field [80]. The theoretical model of this effect must inevitably deal with a strong conventional Hall effect and the strict separation into conventional and anomalous Hall effects may not work anymore, for example due to the phase space volume correction following from wavepacket equations of motion. The theory of the AHE in this regime should be upgraded.

It is worth mentioning that new types of the AHE have been recently proposed for an experimental verification [73, 74, 81, 82] and the semiclassical theory can be used to describe these effects too. There are also suggestions of alternative mechanisms of the AHE and the spin Hall effect based on the possibility of a spin-dependent force [83–85]. This idea so far is based mainly on the Drude-model type of arguments and its verification by rigorous quantum mechanical and numerical techniques still has not been developed.

Finally, an extra numerical and *ab initio* study of the AHE is needed. So far all existing research of this kind concentrated only on the intrinsic contribution, treating discrepancies with experiments by introducing a finite lifetime of quasiparticles [4, 86]. The rigorous numerical study of

the anomalous Hall conductivity in models with a realistic disorder is still missing. In contrast, currently there is a number of successful publications on the related spin Hall effect [87, 88] that demonstrated good agreement with existing theoretical results and enabled their extension to analytically complicated and experimentally more realistic strong disorder cases [89–95]. Such numerical studies were also valuable to understand the problem of the spin accumulation near the edges. Similar research should be very valuable in applications to the AHE. Simple models such as the Rashba coupled 2D electron system with an out-of-plane magnetization should be within the reach of modern numerical algorithms.

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