Intrinsic anomalous Hall effect and local polarizabilities

Pavel Středa[1] and Thibaut Jonckheere[2]
[1]*Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 53 Praha, Czech Republic*
[2]*Faculté de Luminy, Centre de Physique Théorique, Case 907, 13288 Marseille, France*
(Received 29 April 2010; revised manuscript received 13 July 2010; published 7 September 2010)

A theory of the intrinsic anomalous Hall effect, based on the space distribution of the current densities, is presented. Spin-orbit coupling gives rise to a spatial separation of the mass centers, and of the current densities, of the quasiparticle states having opposite group velocities. It is shown that this microscopic property is essential for the existence of the anomalous Hall effect.

DOI: 10.1103/PhysRevB.82.113303 PACS number(s): 72.25.−b, 71.70.Ej, 75.20.−g

It has been known for more than a century that ferromagnetic materials exhibit an extraordinary Hall effect which does not vanish at zero magnetic field. The theory of this so-called anomalous Hall effect (AHE) has a long and confusing history, with different approaches giving in some cases conflicting results. While more recent calculations have somewhat unified the different approaches and clarified the situation, it is still an active topic of research. Recently theories together with number of experimental observations have been reviewed by Nagaosa *et al.*[1] Three broad regimes for anomalous Hall effect have been identified: a high-conductivity regime in which skew scattering dominates, the so-called good metal or intrinsic regime in which anomalous Hall conductivity is roughly independent of scattering and bad metal (or hopping) regime in which Hall conductivity decreases with decreasing of the longitudinal conductivity. All three regimes are nicely illustrated by the dependence of the anomalous Hall conductivity on the longitudinal one for experimental data taken on different materials.[2] It is generally accepted that the anomalous Hall effect is induced by spin-orbit coupling as first suggested by Karplus and Luttinger[3] in 1954. As has been recently argued, it is accompanied by a strong orbital Hall effect.[4–6] Spin-orbit coupling is also responsible for the spin Hall effect, represented by spin accumulation on the edges of a current carrying samples.[7,8]

For the intrinsic, scattering-independent regime the best quantitative agreement with experimental observations has been obtained with semiclassical transport theory,[9] leading to the Berry-phase correction to the group velocity. In this case Hall conductivity is expressed in terms of the Berry-phase curvatures of Bloch states as originally derived by Karplus and Luttinger[3] by the use of the Kubo formula. This result has been obtained by considering linear response to the dynamical force, the electric field. In accord with the general theory of irreversible processes the same result should be obtainable as the response to the statistical force, the gradient of the chemical potential. It is the aim of this report to analyze such type of the response for the intrinsic regime.

Our approach is based on the analysis of the space distribution of local current densities, and it is simple and rather intuitive. We will show that the anomalous Hall conductivity is related to the spatial separation of the mass centers of states with opposite velocities. This confirms the interpretation of AHE in ferromagnetic systems as a consequence of the periodic field of electric dipoles (electric polarizability) induced by the applied current,[3,10,11] despite the fact that the original arguments were not convincing.[12] We will also show that in nonmagnetic systems, the spin-orbit coupling leads to a periodic variation in the spin polarizability of the current densities in the transport regime. This effect can be viewed as an internal spin Hall effect. General consideration will be accompanied by a simple model illustrating the above mentioned local polarizibilities. For the sake of simplicity, we limit our consideration to crystalline structures invariant under space inversion.

Current-density distribution is closely related to the orbital magnetization of solids. In zero magnetic field it has its origin in the orbital magnetic moment of atomic states. Ignoring spin effects, atomic wave functions in spherical polar-coordinate system can be written as

$$\Psi_{\alpha}^{(at)}(r,\theta,\phi) = f_{\alpha}(r,\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}, \quad \alpha \equiv n,l,m, \tag{1}$$

where m is the so-called magnetic quantum number, with $m=0,\pm 1,\cdots$ and $|m|\leq l$. It determines the magnetic moment along the $\hat{z}$ direction

$$M_z(\alpha) \equiv -\frac{e}{2c}\langle\alpha|(\vec{r}\times\vec{v})_z|\alpha\rangle \equiv -\frac{m}{|m|}\frac{\pi R_{\alpha}^2}{c}|j_{\alpha}|, \tag{2}$$

where e denotes absolute value of the electron charge and $\vec{v}$ stands for velocity operator. The last expression represents a classical analogy with j_{α} being the current flowing on a circular loop of the radius R_{α}. Because of the energy degeneracy in m the total orbital magnetic moment vanishes. However, spin-orbit coupling together with exchange interaction remove this degeneracy giving rise to nonzero magnetic moment.

Within a mean-field approach the electron properties are controlled by a single electron Hamiltonian H containing two additive terms H_{so} and H_z representing spin-orbit coupling and an effective Zeeman-type spin splitting due to the exchange interaction, respectively,

$$H = \frac{p^2}{2m_0} + V(\vec{r}) + H_{so} + H_z \tag{3}$$

with m_0 being free-electron mass, $V(\vec{r})$ denotes the crystalline potential, $\vec{p}$ is momentum operator, and

$$H_{so} = \frac{\lambda_c^2}{4\hbar}\vec{\sigma}\cdot[\vec{\nabla}V(\vec{r})\times\vec{p}], \quad H_z = -\mu_B\vec{B}_{\text{eff}}\cdot\vec{\sigma}, \tag{4}$$

where λ_c denotes an effective Compton length and elements of the vector $\vec{\sigma}$ are Pauli matrices. Strength of the Zeeman-type splitting is controlled by the product of the Bohr magneton μ_B and the parameter $\vec{B}_{\text{eff}}$ representing an effective magnetic field. The corresponding velocity operator reads

$$\vec{v} = \frac{\vec{p}}{m_0} + \frac{\lambda_c^2}{4\hbar}\vec{\sigma}\times\vec{\nabla}V(\vec{r}). \tag{5}$$

Eigenfunctions are spinors with two components, and since spin-orbit coupling does not destroy translation symmetry they are of the Bloch form. Energy spectrum $E_\alpha(k)$ is a function of the wave vector $\vec{k}$, with α being a band index, now including also, in addition to atomic-orbital numbers, a spin number. Eigenfunctions are of the following form:

$$|\alpha,\vec{k}\rangle \equiv \Psi_{\alpha,\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{8\pi^3}}u_\alpha(\vec{k},\vec{r}) \tag{6}$$

and velocity expectation values are

$$\vec{v}_\alpha(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E_\alpha(\vec{k}). \tag{7}$$

Spinors $u_\alpha(k,\vec{r})$ are periodic functions of the lattice translation vectors. Assumed invariance under space inversion results in following $\vec{k}$-space symmetry: $E_\alpha(\vec{k})=E_\alpha(-\vec{k})$ and $v_\alpha(\vec{k})=-v_\alpha(-\vec{k})$.

In order to analyze the role of the space distribution of the current densities, it is illustrative to present first the results for a simple model of a linear chain of atomic orbitals. It is assumed that this chain is forming a one-dimensional lattice along the $\hat{x}$ direction with a period a. Model parameter will be chosen to satisfy conditions for which the tight-binding approach is applicable. Energy bands originated in overlap of atomic states $|\alpha\rangle$ will be denoted by the corresponding magnetic quantum number m. To model a ferromagnetic state, we assume that the effective field $\vec{B}_{\text{eff}}$ is parallel with $\hat{z}$ direction and energy bands are fully spin polarized, with $s_z=\pm 1/2$ being a good quantum number. We have obtained numerical results by diagonalizing the single-particle Hamiltonian for a two-dimensional separable chain potential

$$V(x,y) = -V_0\cos(2\pi x/a) + m_0\Omega_0^2 y^2/2. \tag{8}$$

Note that adding a z-dependent potential would not affect the current distribution of the considered model system. The parameters have been chosen to be in the tight-binding regime, i.e., to fully separate the studied band from the other energy bands (we used $2m_0a^2V_0/\hbar^2=75.0$, $m_0\Omega_0^2a^2=1.4\times 4\pi^2V_0$, and $\pi\lambda_c^2/a^2=0.015$).

Typical current-density distribution within the unit cell for the Bloch states $|\alpha,k_x\rangle$ and $|\alpha,-k_x\rangle$ are shown in Figs. 1(a) and 1(b), respectively. One observes circulating currents forming vortices, which have the same orientation for both cases. This orientation coincides with the orientation of the circulating current of the atomic orbitals. In addition to this circulating current, there is a direct current flow, with opposite sign for the two cases. Corresponding total current and its direction is just determined by the velocity expectation value, $-ev_x^\alpha(k_x)$. Note that these current flows are spatially separated in the two cases (they are on opposite sides of the circulating current). The current densities averaged over x and z coordinates,

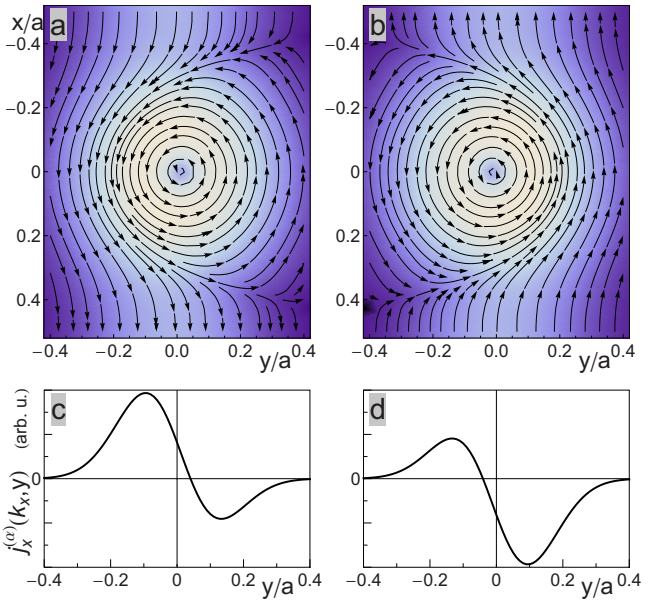

FIG. 1. (Color online) Current distributions for an energy band given by a chain of atomic states with spin $s_z=1/2$ and $m=-1$ for [(a) and (c)] $k_x=1.5/a$ and [(b) and (d)] $k_x=-1.5/a$. In (a) and (b), the arrows indicate the direction of the current and a lighter background indicates a larger current. In (c) and (d), the averaged current densities $j_x^\alpha(k_x,y)$ are shown.

$$j_x^\alpha(k_x,y) = -e\int\int \Psi_{\alpha,k_x}^+(\vec{r})v_x\Psi_{\alpha,k_x}(\vec{r})dxdz, \tag{9}$$

clearly demonstrate the above-mentioned spatial separation of the currents having opposite velocity directions, as shown in Figs. 1(c) and 1(d).

This space separation of currents flowing in opposite directions is closely related to the mass-center separation $\Delta Y_\alpha(k_x)$ of states $|\alpha,k_x\rangle$ and $|\alpha,-k_x\rangle$ with k_x being consider as positive, $k_x>0$. For the considered model potential, Eq. (8), the y component of the force operator reads

$$F_y \equiv \frac{1}{i\hbar}[p_y,H] = -m_0\Omega_0^2 y + 2s_z\frac{\lambda_c^2}{4\hbar}m_0\Omega_0^2 p_x. \tag{10}$$

In a stationary state the force expectation values has to vanish. Using the relation between p_x and v_x given by Eq. (5) we get

$$\Delta Y_\alpha(k_x) = 2s_z\frac{\lambda_c^2 m_0}{4\hbar}\left[1-\left(\frac{\lambda_c^2 m_0}{4\hbar}\right)^2\Omega_0^2\right]^{-1}2v_x^\alpha(k_x). \tag{11}$$

In the limiting case of vanishing spin-orbit coupling $\Delta Y_\alpha(k_x)\to 0$ and sum of the current densities $j_x^\alpha(k_x,y)+j_x^\alpha(-k_x,y)$ approaches zero as well.

Nonzero total current appears if there is different occupation of states with opposite velocities which can be characterized by the chemical-potential difference $\Delta\mu$. It can be related to the electric field along the $\hat{y}$ direction, $\mathcal{E}_y = \Delta\mu/(e|\Delta Y_\alpha(k_F)|)$, with $\Delta Y_\alpha(k_F)$ being the mass-center separation of quasiparticles having opposite velocities at the Fermi energy $E_F=\mu$. Within linear-response approach the resulting current at zero temperature reads

$$J_x^\alpha(\mu) = -\frac{e}{h}\frac{v_x^\alpha(k_F) - v_x^\alpha(-k_F)}{|v_x^\alpha(k_F)|}\Delta\mu = -\frac{e^2}{h}\Delta Y_\alpha(k_F)\mathcal{E}_y. \tag{12}$$

Because of the nonzero separation $\Delta Y_\alpha(k_F)$ and nonequal occupation of states with opposite velocities the applied current is giving rise an electric dipole moment, i.e., a charge polarization is induced.

For the later use, let us express current $J_x^\alpha(\mu)$ in terms of the following quantity:

$$\frac{\vec{P}_\alpha(\vec{k})}{\Omega_{\rm ws}} \equiv -\frac{e}{c}\langle\alpha,\vec{k}|\vec{r}|\alpha,\vec{k}\rangle \times \vec{v}_\alpha(\vec{k}), \tag{13}$$

where $\Omega_{\rm ws}$ defines a unit-cell volume. Evaluation of the following expression:

$$J_x^\alpha(\mu) = -\frac{ec\mathcal{E}_y}{2\pi\Omega_{\rm ws}}\int_{-\pi}^{+\pi}\delta(E_\alpha(k_x)-\mu)[\vec{P}_\alpha(k_x)]_z dk_x \tag{14}$$

immediately gives the above result, Eq. (12) (using $\Omega_{\rm ws}=a$ for the linear chain of atomic orbitals) since velocity expectation value along the $\hat{y}$ direction vanishes. The above defined quantity, Eq. (13), is the part of the orbital magnetic moment within each of the unit cells which gives rise to an electric dipole moment in the current carrying regime. For this reason it will be called as the orbital polarization moment.

Generalization of the above treatment to a three-dimensional system is straightforward. Velocity expectation values have nonzero component also along the $\hat{y}$ direction and they contribute to the orbital polarization moment defined by Eq. (13). The resulting contribution of the band α to the Hall conductivity component σ_{xy} can thus be written as follows:

$$\sigma_{xy}^{(\alpha)}(\mu) = -\frac{ec}{8\pi^3\Omega_{\rm ws}}\int_{\rm BZ}\delta(E_\alpha(\vec{k})-\mu)[\vec{P}_\alpha(\vec{k})]_z d^3k, \tag{15}$$

where integration is limited to the Brillouin zone and $\Omega_{\rm ws}$ now denotes volume of the Wiegner-Seitz cell. Inserting for $\vec{P}_\alpha(\vec{k})$ and $\vec{v}_\alpha(\vec{k})$ their explicit forms, Eq. (13) and Eq. (7), respectively, and using equality

$$\langle\alpha,\vec{k}|\vec{r}|\alpha,\vec{k}\rangle = -\,{\rm Im}\int_{\Omega_{\rm ws}} u_\alpha^+(\vec{k},\vec{r})[\vec{\nabla}_{\vec{k}}u_\alpha(\vec{k},\vec{r})]d^3r, \tag{16}$$

already derived by Karplus and Luttinger,[3] the integration per parts gives the well-known expression for the Hall conductivity of Bloch electrons

$$\sigma_{xy}(\mu) = -\frac{e^2}{4\pi^2 h}\sum_\alpha\int_{\rm BZ} f_0(E_\alpha(\vec{k}))[\vec{\Omega}_\alpha(\vec{k})]_z d^3k. \tag{17}$$

Here $f_0(E)$ stands for zero-temperature Fermi-Dirac distribution function and the Berry-phase curvature $\vec{\Omega}_\alpha(\vec{k})$ defined using the periodic part of Bloch functions, $u_\alpha(\vec{k},\vec{r})$, reads

$$\vec{\Omega}_\alpha(\vec{k}) = -\,{\rm Im}\langle\vec{\nabla}_{\vec{k}}u_\alpha(\vec{k},\vec{r})| \times |\vec{\nabla}_{\vec{k}}u_\alpha(\vec{k},\vec{r})\rangle. \tag{18}$$

Our description of the anomalous Hall effect based on charge polarization effect is thus equivalent to the approach based on the Berry-phase correction.[9] The orbital polarization moment we introduced is equivalent to the Berry-phase correction to the orbital magnetization.[13]

For completeness, we must note that for the three-dimensional case, computing the current distribution, say along the $\hat{y}$ direction, as well as the quantity ΔY defining the local dipole moments induced in transport regime is not trivial. It requires to express eigenfunctions in a mixed representation, to preserve the Bloch form along the $\hat{x}$ direction, while using Wannier representation along perpendicular directions. The Wannier representation gives functions which are bounded along the $\hat{y}$ direction, allowing to compute ΔY. Nevertheless, qualitative features of both quantities are not affected by system dimensionality.

Discussed relation between the anomalous Hall effect and the local charge polarization is similar to that obtained for Hall conductivity of Bloch electrons in rational quantizing magnetic fields in terms of charge polarization.[14,15] However, in that case the physical picture is strongly affected by chiral magnetic edge states.

Assumed nonequal occupation of states having different velocities is controlled by electron transitions between them. Such transitions are due to the scattering which is naturally of the side-jump character since mass-center positions of states with different $\vec{k}$ are different. This type of scattering does not affect the Hall conductivity which is given as the sum of the additive band contributions defined by Eq. (15) or Eq. (17). However, this view can only be applied to the good metal regime for which anomalous Hall conductivity is roughly scattering independent quantity. It does not include hopping regime for which disorder is so strong that eigenfunctions cannot be further considered to have Bloch character. Also skew scattering is ignored which excludes applicability to high-conductivity regime.

Of particular interest are nonmagnetic systems in which spin-orbit coupling is not negligible but effective Zeeman-type spin splitting vanishes, $B_{\rm eff}\to 0$. We have on mind systems in which applied current does not induce Hall voltage but there appears spin accumulation on sample edges. Typical example is GaAs on which such effect was first observed.[7,8] Local properties of such systems can be illustrated by using the above defined model of the single atomic chain assuming twofold band degeneracy. In the case of the vanishing Zeeman-type splitting states $|\alpha,k_x\rangle$ with orbital number m and spin s_z are of the same energy as states $|\bar{\alpha},k_x\rangle$ with opposite sign of the orbital number and spin, $-m$ and $-s_z$. Their orbital magnetizations have opposite sign, the sum of their current densities vanishes, $j_x^\alpha(k_x,y)+j_x^{\bar{\alpha}}(k_x,y)$

$+j_x^{\alpha}(-k_x,y)+j_x^{\bar{\alpha}}(-k_x,y)=0$, and total magnetization vanishes as well. The mass-center separation has also opposite signs, $\Delta Y_{\alpha}(k_x)=-\Delta Y_{\bar{\alpha}}(k_x)$, and in accord with Eq. (12) the resulting anomalous Hall effect vanishes.

However, the spin-orbit coupling has still an important effect in the transport regime. The current applied along the $\hat{x}$ direction gives rise for each band to nonequal occupation of states with opposite velocities represented by a local chemical-potential difference $\Delta\mu$. The two considered bands contribute by the same current but their Fermi energy states have different space distribution because of the different mass-center positions determined by their spin orientation, Eq. (11). As a result, the spin polarization of the transport current density averaged over x and z coordinates will be a function of the y coordinate. This is illustrated in Fig. 2, where the averaged transport current densities are shown for the same model parameters as in Fig. 1. Qualitatively the same features are expected for three-dimensional crystals, i.e., that the spin polarization of the transport current density will show a periodic oscillation. This property can be interpreted as an internal spin Hall effect.

To conclude, we have shown that the mass-center separation as well as the current-density separation of states having opposite velocities is a typical feature of the systems with spin-orbit coupling. In the transport regime it gives rise to the charge polarization inducing anomalous Hall effect in ferromagnetic crystals. We have shown that this intuitive picture gives the same results as the approach based on the Berry-phase correction. Furthermore, in nonmagnetic systems it leads to a periodic spatial variation in the spin polarizability of the transport current density, a prediction we called "internal spin Hall effect."

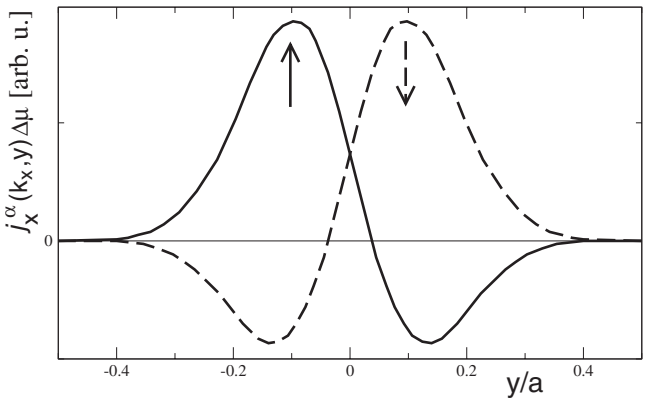

FIG. 2. Transport current densities $j_x^{\alpha}(k_x,y)\Delta\mu$ for the energy band of the twofold degeneracy ($B_{\text{eff}}=0$) given by a chain of atomic states $|\alpha\rangle$ with $m=-1$, $s_z=1/2$ (full line) and $m=1$, $s_z=-1/2$ (dashed line) for Fermi energy given by the wave number $k_x=1.5/a$.

The authors acknowledge support from Grant Agency of the Czech Republic (Grant No. 202/08/0551) and the Institutional Research Plan No. AV0Z10100521. P.S. thanks CPT (UMR 6207 of CNRS) and Université du Sud Toulon-Var for their hospitality.

[1] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys. **82**, 1539 (2010).
[2] T. Miyasato, N. Abe, T. Fujii, A. Asamitsu, S. Onoda, Y. Onose, N. Nagaosa, and Y. Tokura, Phys. Rev. Lett. **99**, 086602 (2007).
[3] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).
[4] R. Shindou and N. Nagaosa, Phys. Rev. Lett. **87**, 116801 (2001).
[5] H. Kontani, T. Tanaka, D. S. Hirashima, K. Yamada, and J. Inoue, Phys. Rev. Lett. **100**, 096601 (2008).
[6] D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B **74**, 024408 (2006).
[7] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science **306**, 1910 (2004).
[8] J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. **94**, 047204 (2005).
[9] G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).
[10] E. N. Adams and E. I. Blount, J. Phys. Chem. Solids **10**, 286 (1959).
[11] R. C. Fivaz, Phys. Rev. **183**, 586 (1969).
[12] L. Berger, Phys. Rev. B **2**, 4559 (1970).
[13] D. Xiao, Y. Yao, Z. Fang, and Q. Niu, Phys. Rev. Lett. **97**, 026603 (2006).
[14] P. Středa, T. Jonckheere, and J. Kučera, Phys. Rev. B **76**, 085310 (2007).
[15] P. Středa, T. Jonckheere, and T. Martin, Phys. Rev. Lett. **100**, 146804 (2008).