Anomalous Hall conductivity: Local orbitals approach

Pavel Středa
Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 53 Praha, Czech Republic
(Received 12 March 2010; revised manuscript received 24 June 2010; published 20 July 2010; publisher error corrected 22 July 2010)

A quantum linear-response theory of the anomalous Hall conductivity based on the properties of single-site orbitals is presented. Effect of the finite-electron lifetime is modeled by energy fluctuations of atomic-like orbitals. Transition from the ideal Bloch system for which the conductivity is determined by the Berry-phase curvatures to the case of strong disorder for which the conductivity becomes dependent on the relaxation time is analyzed. Presented tight-binding model gives by the unified way experimentally observed qualitative features of the anomalous conductivity in the so-called good metal regime and that called as bad metal or hopping regime.

DOI: 10.1103/PhysRevB.82.045115 PACS number(s): 71.70.Ej, 72.10.Bg, 72.80.Ga

I. INTRODUCTION

It has been known for more than a century that ferromagnetic materials exhibit, in addition to the standard Hall effect when placed in a magnetic field, an extraordinary Hall effect which does not vanish at zero magnetic field. The theory of this so-called anomalous Hall effect 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, see, for example, the recent review by Nagaosa *et al.*[1]

It is generally accepted that anomalous Hall effect is induced by spin-orbit coupling. It was first suggested by Karplus and Luttinger[2] in 1954 to explain anomalous Hall effect observed on ferromagnetic crystals. Their analysis leads to the scattering-independent off-diagonal components of the conductivity, which are attributed to the so-called "intrinsic" effect. Later, theories of this effect based on several specific models have been developed.[3,4] As shown recently, it is accompanied by a strong orbital Hall effect.[5,6] The conductivity is affected by scattering, which in the presence of spin-orbit coupling is basically of two types, the so-called side-jump[7] and skew scattering.[8–10] They also lead to an anomalous Hall effect, called "extrinsic." It has also been argued that in the anomalous Hall regime a periodic field of electric dipoles (electric polarizability) is induced by the applied current.[2,11,12] This property has recently been shown to be related to the so-called orbital polarization moment[13] which is determined by Berry-phase curvature in pure systems.[14]

The best quantitative agreement with experimental observations has been obtained by semiclassical transport theory,[14] leading to the Berry-phase correction to the group velocity. For Fe crystals[15] it yields an anomalous conductivity $\sim 750\ \Omega^{-1}\ \mathrm{cm}^{-1}$ while a value approaching $1000\ \Omega^{-1}\ \mathrm{cm}^{-1}$ has been observed. However, up to now, generalization of this theory to systems with strong disorder or subject to other types of fluctuations seemed to fail. It is the main aim of this paper to present theoretical treatment filling this gap.

In contrast to standard transport theories the Hall conductivity is expressed in terms of local atomic-like orbitals. It is explicitly derived that for perfect Bloch electron systems this description coincides with that given by Berry-phase curvatures indicating intrinsic, topological, origin of anomalous Hall effect. Presented view based on atomic-like orbitals allows to include effect of disorder by a local energy fluctuation of these orbitals which is an alternative description of scattering events. Fluctuations modify the Hall conductivity and transition from perfect to strongly disordered systems is analyzed. So-called intrinsic and extrinsic Hall effect are just treated by an unified way. To test presented view based on local atomic-like orbitals the two-band model within tight-binding approach is used. Obtained dependence of the anomalous Hall conductivity on the relaxation time shows the observed qualitative features.[1,16] Similar features has also been obtained by the different procedure with relaxation time being a fitting parameter.[17] In contrast to this work the presented model allows to relate relaxation time to fluctuations of atomic-like orbitals, i.e., to its microscopic origin. By the unified way it gives experimentally observed scaling of anomalous Hall conductivity σ_{xy} with diagonal conductivity component σ_{xx} in the region of the so-called good metal for which $\sigma_{xy} \sim (\sigma_{xx})^0$ and that of the bad metal for which $\sigma_{xy} \sim (\sigma_{xx})^{1.6}$.

The paper is organized as follows. In Sec. II basic properties of electron systems in crystalline structures with spin-orbit coupling are summarized while basic expressions for Hall conductivity derived by using the quantum linear-response theory are rederived in Sec. III. In Sec. IV an alternative expression for Hall conductivity, including on-energy shell matrix elements only, is derived. Section V is devoted to perfect Bloch electron systems where conductivity is expressed in terms of local orbital polarization moments which are further expressed via the Berry-phase curvature. In Sec. VI a two-band model in tight-binding approach is presented to estimate the effect of a finite-electron lifetime to the anomalous Hall conductivity at zero magnetic field. Presented theory of anomalous Hall effect is summarized and commented in the last section.

II. SINGLE-ELECTRON HAMILTONIAN AND STATISTICAL FLUCTUATIONS

Within a mean-field approach, electron properties are controlled by a single-electron Hamiltonian which we consider in the following standard form:

 ©2010 The American Physical Society

$$H = \frac{\vec{p}^2}{2m_0} + V(\vec{r}) + \frac{\lambda_c^2}{4\hbar}\vec{\sigma}\cdot[\vec{\nabla}V(\vec{r})\times\vec{p}] - \mu_B\vec{B}_{\rm eff}\cdot\vec{\sigma}. \quad (1)$$

Here, m_0 and μ_B denote free-electron mass and the Bohr magneton, respectively, $\vec{p}$ is the momentum operator, $V(\vec{r})$ denotes a background potential, and components of $\vec{\sigma}$ are Pauli matrices. The third term on the right-hand side represents spin-orbit coupling with λ_c being an effective Compton length. The last term on the right-hand side describes Zeeman-type spin splitting due to the exchange-correlation energy represented by an effective field $\vec{B}_{\rm eff}$ which can generally be position dependent. The corresponding velocity operator reads

$$\vec{v} = \frac{1}{i\hbar}[\vec{r},H] = \frac{\vec{p}}{m_0} + \frac{\lambda_c^2}{4\hbar}\vec{\sigma}\times\vec{\nabla}V(\vec{r}). \quad (2)$$

Strictly speaking, Hamiltonian H quite well defines properties of electrons located within a finite volume of characteristic dimensions defined by the electron coherence length. Within each of such volumes the background potential as well $\vec{B}_{\rm eff}$ can be different. This way, a set of electron systems, the statistical ensemble, is defined. If time-dependent fluctuations can be treated within an adiabatic approach,[18] they can also be included in this ensemble. However, we should have in mind that such type of fluctuations, e.g., lattice vibrations, affects size of the coherent regions. Measurable quantities are given by their statistically averaged values. It is useful to split Hamiltonian H, Eq. (1), into two parts

$$H = H_0 + \delta H, \quad H_0 \equiv \langle H\rangle_{\rm av}, \quad (3)$$

where only δH depends on statistical fluctuations. For crystalline solids, to which the present treatment is devoted, statistically averaged Hamiltonian H_0, obeys full crystal symmetry and the effective field $\vec{B}_{\rm eff}$ can be assumed constant. It defines the so-called virtual crystal with eigenstates $|n,\vec{k}\rangle$ of the energy $E_n(\vec{k})$, characterized by the band index n and the wave vector $\vec{k}$. Eigenfunctions are two-component Bloch spinors,

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

$$H_0|n,\vec{k}\rangle \equiv \langle H\rangle_{\rm av}|n,\vec{k}\rangle = E_n(\vec{k})|n,\vec{k}\rangle, \quad (4)$$

where $u_{n,\vec{k}}(\vec{r})$ are spinor functions periodic in $\vec{r}$ with period defined by the elementary lattice translations. Velocity matrix elements are diagonal in the wave vector $\vec{k}$ located within the Brillouin zone,

$$\langle n,\vec{k}|\vec{v}|n',\vec{k}'\rangle = \vec{v}^{n,n'}(\vec{k})\delta_{\vec{k},\vec{k}'} \quad (5)$$

and the expectation values read

$$\vec{v}_n(\vec{k}) \equiv \langle n,\vec{k}|\vec{v}|n,\vec{k}\rangle = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}E_n(\vec{k}). \quad (6)$$

Equilibrium properties are determined by the effective Hamiltonian, $H_{\rm eff}$, defined by the statistically averaged Green's function,[19]

$$\langle G(z)\rangle_{\rm av} \equiv \left\langle \frac{1}{z-H}\right\rangle_{\rm av} \equiv \frac{1}{z-H_{\rm eff}(z)}, \quad (7)$$

where z is the complex energy variable. It has the full crystal symmetry and it is diagonal in the representation given by eigenstates of the averaged Hamiltonian H_0, Eq. (4). Effective Hamiltonian is non-Hermitian and energy dependent but it is analytic in both complex half planes, $H_{\rm eff}(z^*)=H_{\rm eff}^{+}(z)$. Its standard form reads

$$H_{\rm eff}(z) = H_0 + \Sigma(z), \quad \Sigma(z) = \Delta(z) - i\Gamma(z), \quad (8)$$

where $\Sigma(z)$ is the energy-dependent self-energy. Inverse value of its imaginary part represents a finite-electron lifetime.

To include an external magnetic field $\vec{B}$ the Hamiltonian defined by Eq. (1) has to be modified. Both the momentum operator entering the Hamiltonian, and the velocity operator, Eq. (2), have to be replaced by their counterparts, which include a vector potential $\vec{A}$,

$$\vec{p} \to \vec{p} + e\vec{A}. \quad (9)$$

Here, e denotes the electron charge absolute value and the magnetic field is given as $\vec{B}=\mathrm{curl}\,\vec{A}$. Also the value of the parameter $\vec{B}_{\rm eff}$ defining Zeeman-type splitting is modified by $\vec{B}$. The external magnetic field generally removes translation symmetry. Exceptions are the so-called rational magnetic fields for which the problem becomes invariant under translations with different elementary translations than those given by the periodic potential.

III. LINEAR-RESPONSE THEORY

In this section the standard linear-response theory will be described and well-known general formulas derived to summarize basic theoretical assumptions. In accord with the original work by Kubo[20] the external electric field is supposed to be turned on at the time $t\to-\infty$ and reach the final value $\vec{\mathcal{E}}$ at $t=0$. Exponential time evolution is considered, $\vec{\mathcal{E}}(t)=\vec{\mathcal{E}}e^{\epsilon t/\hbar}$, with $\epsilon>0$ being an infinitesimally small quantity. It gives rise to the Hamiltonian perturbation $e\vec{r}\cdot\vec{\mathcal{E}}(t)$ and corresponding density matrix $\rho(t)$ has to satisfy the equation of motion which reads

$$\frac{\partial\rho(t)}{\partial t} + \frac{1}{i\hbar}[\rho(t),H + e\vec{r}\cdot\vec{\mathcal{E}}(t)] = 0. \quad (10)$$

It can be written in the following way:

$$\rho(t) = \rho_0(H) + e^{-iHt/\hbar}\rho_1(t)e^{iHt/\hbar}, \quad (11)$$

where $\rho_1(t)$ represents the deviation from the density matrix in the absence of electric field given by the Fermi-Dirac distribution function,

$$\rho_0(H) = (1 + e^{(H-\mu)/k_BT})^{-1}, \quad (12)$$

where μ and k_BT are the chemical potential and thermal energy, respectively. Up to linear terms in the electric field, $\rho_1(t)$ reaches the following value at $t=0$,

$$\rho_1(0) = \frac{i}{\hbar}\int_0^{+\infty} e^{-\epsilon t/\hbar} e^{-iHt/\hbar}[\rho_0(H), e\vec{r}\cdot\vec{\mathcal{E}}]e^{iHt/\hbar}dt \quad (13)$$

and the resulting current density reads

$$\vec{j} = -e \lim_{\epsilon\to 0^+} \langle \mathrm{Tr}[\rho_1(0)\vec{v}]\rangle_{\mathrm{av}}. \quad (14)$$

Generally, the potential perturbation $e\vec{\mathcal{E}}\vec{r}$ of the Hamiltonian is not the only perturbation caused by electric field. The potential gradient $e\vec{\mathcal{E}}$ enters the spin-orbit term of the Hamiltonian, Eq. (1), as well as the velocity operator, Eq. (2), giving rise to additive terms linear in electric field. Resulting contributions to the current density are of a higher order than λ_c^2 in the Compton length. For the considered Hamiltonian H, Eq. (1), which includes spin-orbit coupling only approximately up to the order of λ_c^2, these contributions thus have to be ignored.

Introducing the δ-function operator,

$$\delta(\eta - H) = -\lim_{\epsilon\to 0^+} \frac{G^+(\eta) - G^-(\eta)}{2\pi i},$$

$$G^{\pm}(\eta) = \frac{1}{\eta - H \pm i\epsilon}, \quad (15)$$

the time integration, Eq. (13), can easily be performed. For the limiting case of the zero temperature in function $\rho_0(H)$ the components of the conductivity tensor obey the following form:

$$\sigma_{ij}(\mu) \equiv \frac{j_i}{\mathcal{E}_j} = -e^2\int_{-\infty}^{\mu} \langle \mathrm{Tr}\{\delta(\eta - H)[v_i G^+ r_j + r_j G^- v_i]\}\rangle_{\mathrm{av}} d\eta, \quad (16)$$

where $i,j=x,y,z$. The proper way to treat the limits in Eq. (14) (due to the electric field time evolution) and Eq. (15) [regularization of $\delta(H-\eta)$] would be to introduce two different infinitesimal parameters and treat both of them independently, after all other steps are taken. However, our procedure of statistical averaging yields a nonzero imaginary part of the self-energy, Γ, entering both averaged operators. Limiting case of the fully coherent system is thus defined by the physically acceptable limit $\Gamma\to 0^+$. That is why it is sufficient to consider just one infinitesimally small parameter $\epsilon\to 0^+$ implicitly entering Eq. (16). Misunderstanding of this limit has been reason for doubts concerning validity of resulting expressions, especially of the Hall conductivity.

The nonzero temperature smearing effect of the distribution function yields

$$\sigma_{ij}(\mu,T) = -\int_{-\infty}^{+\infty} \frac{d\rho_0(\eta)}{d\eta}\sigma_{ij}(\eta)d\eta. \quad (17)$$

This relation allows to limit our attention to the analysis of the energy-dependent conductivity given by Eq. (16). It does not mean that $\sigma_{ij}(\mu)$ has to be temperature independent since potential fluctuations as well as some of the Hamiltonian parameters can be implicitly temperature-dependent quantities, as is, for example, $\vec{B}_{\mathrm{eff}}$ representing the exchange-interaction effect.

Using definition of the velocity operator,

$$\vec{v} = \frac{1}{i\hbar}[\vec{r},H] = -\frac{1}{i\hbar}\{\vec{r},[G^{\pm}(\eta)]^{-1}\} \quad (18)$$

and the identity

$$[G^{\pm}(\eta)]^2 = -\frac{dG^{\pm}}{d\eta}, \quad (19)$$

the Eq. (16) can be rewritten[21] in a form including velocity operators only,

$$\sigma_{ij}(\mu) = i\hbar e^2\int_{-\infty}^{\mu} \left\langle \mathrm{Tr}\left\{\delta(\eta - H)\left[v_i\frac{dG^+}{d\eta}v_j - v_j\frac{dG^-}{d\eta}v_i\right]\right\}\right\rangle_{\mathrm{av}} d\eta. \quad (20)$$

It coincides with that obtained by Bastin *et al.*[22] by the use of a different procedure. For diagonal components of the conductivity tensor the integration by parts gives the well known Kubo-Greenwood formula,[23]

$$\sigma_{ii}(\mu) = \pi e^2\hbar\langle \mathrm{Tr}\{v_i\delta(\mu - H)v_i\delta(\mu - H)\}\rangle_{\mathrm{av}}. \quad (21)$$

Making use of the following identity:[21,24]

$$i\hbar\,\mathrm{Tr}\left\{\delta(\eta - H)\left[v_i\frac{dG^+}{d\eta}v_j - v_j\frac{dG^-}{d\eta}v_i\right]\right\} = \frac{i\hbar}{2}\frac{d}{d\eta}\mathrm{Tr}\{\delta(\eta - H)[v_i G^+(\eta)v_j - v_j G^-(\eta)v_i]\} + \frac{1}{2}\frac{d}{d\eta}\mathrm{Tr}\{\delta(\eta - H)[r_i v_j - r_j v_i]\}, \quad (22)$$

the off-diagonal conductivity components can be split into two parts,[25]

$$\sigma_{xy}(\mu) = \sigma_{xy}^{(\mathrm{I})}(\mu) + \sigma_{xy}^{(\mathrm{II})}(\mu) = -\sigma_{yx}(\mu), \tag{23}$$

where

$$\sigma_{xy}^{(\mathrm{I})}(\mu) = e^2\frac{i\hbar}{2}\langle \mathrm{Tr}\{\delta(\mu - H)[v_x G^+(\mu) v_y - v_y G^-(\mu) v_x]\}\rangle_{\mathrm{av}} \tag{24}$$

and

$$\sigma_{xy}^{(\mathrm{II})}(\mu) = \frac{e^2}{2}\langle \mathrm{Tr}\{\delta(\mu - H)[x v_y - y v_x]\}\rangle_{\mathrm{av}} = -e^2\langle \mathrm{Tr}\{\delta(\eta - H) y v_x\}\rangle_{\mathrm{av}}. \tag{25}$$

These conductivity formulas are quite general, they include both the effect of the magnetic field and the spin-orbit coupling[26] since for derivation only general definition of the velocity operator, Eq. (18), has been used. Similar treatment, but formally more complicated, is applicable to other transport coefficients, such as the thermopower and the heat conductivity, allowing to express them via components of the conductivity tensor.[24] For example, the transverse Peltier coefficient of ferromagnetic metals is determined by the energy dependence of the anomalous Hall conductivity. Under the standard conditions their relation satisfies the Mott rule as has already been experimentally verified.[16]

The above expressions for the Hall conductivity $\sigma_{xy}(\mu)$ have been particularly useful for understanding of the quantum-Hall effect. While the contribution $\sigma_{xy}^{(\mathrm{I})}(\mu)$, called as Fermi-surface term, vanishes whenever μ is located within an energy gap, the contribution $\sigma_{xy}^{(\mathrm{II})}(\mu)$, called as Fermi-sea term, can remain finite giving rise to quantized values of the Hall conductivity.[25] Fermi-surface term $\sigma_{xy}^{(\mathrm{I})}(\mu)$ does not vanish if the Fermi energy is located within an energy band or even if it is within the region of localized states. In the later case it is just canceled by the contribution of localized states to the Fermi-sea term, $\sigma_{xy}^{(\mathrm{II})}(\mu)$, and the resulting total Hall conductivity is thus not affected by localized states. Similarly, in the case of the Fermi energy located within an energy band a non-negligible part of $\sigma_{xy}^{(\mathrm{I})}(\mu)$ is nearly canceled by part of the $\sigma_{xy}^{(\mathrm{II})}(\mu)$.[17,27] It should be thus useful to derive an alternative form of the expression for the Hall conductivity suitable for a clear physical interpretation.

IV. HALL CONDUCTIVITY IN TERMS OF ON-ENERGY-SHELL MATRIX ELEMENTS

Conductivity can directly be measured on samples with so-called Corbino disk geometry. In the limiting case of the large disk radii such samples can be approximated by strips with a rectangular cross section $L_y L_z$. Using a proper choice of the vector potential, periodic boundary conditions along $\hat{x}$ direction can be considered on the length L_x. This geometry allows to apply an electric field along $\hat{y}$ direction, and establish σ_{yy}, and also the Hall current along $\hat{y}$ direction and consequently σ_{xy}. Under these boundary conditions the eigenvalue problem for one particular Hamiltonian of the form given by Eq. (1) can be solved, at least, in principle. Obtained eigenstates $|\alpha\rangle$ of energy E_α represent one of the systems belonging to the considered statistical ensemble. A corresponding contribution to the Hall conductivity can be analyzed by using this α representation.

The term given by Eq. (24) reads

$$\sigma_{xy}^{(\mathrm{I})}(\alpha,E) = e^2\frac{i\hbar}{2}\sum_{\alpha,\alpha'}\delta(E - E_\alpha) \times [v_x^{\alpha,\alpha'} G_{\alpha'}^+(E) v_y^{\alpha',\alpha} - v_y^{\alpha,\alpha'} G_{\alpha'}^-(E) v_x^{\alpha',\alpha}], \tag{26}$$

where $v_{x,y}^{\alpha,\alpha'}$ denotes velocity matrix elements. Inserting commutation relation, Eq. (18), for the operator v_y, we get

$$\sigma_{xy}^{(\mathrm{I})}(\alpha,E) = \frac{e^2}{2}\sum_{\alpha,\alpha'}\delta(E - E_\alpha)(E_\alpha - E_{\alpha'}) \times \left[\frac{v_x^{\alpha,\alpha'} y^{\alpha',\alpha}}{E - E_{\alpha'} + i\epsilon} + \frac{y^{\alpha,\alpha'} v_x^{\alpha',\alpha}}{E - E_{\alpha'} - i\epsilon}\right]. \tag{27}$$

Note that because of the considered strip geometry, matrix elements of the y coordinate are finite. Since terms for which $E_\alpha = E_{\alpha'}$ vanish, we get

$$\sigma_{xy}^{(\mathrm{I})}(\alpha,E) = \frac{e^2}{2}\sum_{\alpha,\alpha'}\delta(E - E_\alpha) \times [v_x^{\alpha,\alpha'} y^{\alpha',\alpha} + y^{\alpha,\alpha'} v_x^{\alpha',\alpha}](1 - \delta_{E_{\alpha'},E_\alpha}). \tag{28}$$

In α representation the remaining conductivity contribution given by Eq. (25) can be written as

$$\sigma_{xy}^{(\mathrm{II})}(\alpha,E) = -\frac{e^2}{2}\sum_{\alpha,\alpha'}\delta(E - E_\alpha) \times [v_x^{\alpha,\alpha'} y^{\alpha',\alpha} + y^{\alpha,\alpha'} v_x^{\alpha',\alpha}]. \tag{29}$$

Sum of $\sigma_{xy}^{(\mathrm{I})}$ and $\sigma_{xy}^{(\mathrm{II})}$ yields the Hall conductivity expressed in terms of on-energy-shell matrix elements only,

$$\sigma_{xy}(E) = -e^2\left\langle \sum_{\alpha,\alpha'}\delta(E - E_\alpha) v_x^{\alpha,\alpha'} y^{\alpha',\alpha}\delta_{E_{\alpha'},E_\alpha}\right\rangle_{\mathrm{av}}, \tag{30}$$

where averaging is taken over the α representations of all elements of the considered ensemble. In the case that the electron system is fully coherent within the considered sample volume $L_x L_y L_z$, the averaging procedure has to be avoided. Energy dissipation take place within electrical contacts while inside the sample it vanishes, $\Gamma \to 0$.

The above expression for the Hall conductivity, Eq. (30), has clear interpretation for quantum-Hall effect. Let us assume that the Fermi energy is located within region of localized states. From their definition only diagonal matrix elements of the y coordinate can differ from zero, $y^{\alpha',\alpha} = y^{\alpha,\alpha}\delta_{\alpha',\alpha}$. Since their velocity expectation values vanish, contribution of localized states to the Hall conductivity van-

ishes as has to be. Nonzero contribution can only be given by chiral edge states giving rise to quantum-Hall effect nonaffected by the presence of localized states.

V. PERFECT BLOCH ELECTRON SYSTEMS

It is of particular interest to apply expression for the Hall conductivity, Eq. (30), to systems having translation symmetry, including those modified by rational magnetic fields. The basic property of these systems is that the velocity matrix elements are diagonal in wave vector $\vec{k}$, Eq. (5). In general, the probability to find on the Fermi-surface states having the same $\vec{k}$ but belonging to different bands is statistically negligible, except of the trivial case of band degeneracy. Since Eq. (30) includes only on-energy-shell matrix elements, interband matrix elements do not affect conductivity of ideal Bloch electron systems.

To proceed further, let us first discuss the contribution to the Hall conductivity, Eq. (30), of states having zero velocity expectation value along $\hat{y}$ direction. It is given by

$$eV_{\rm ws}[v_x^{n,n}(\vec{k})y_n(\vec{k}) + v_x^{n,n}(-\vec{k})y_n(-\vec{k})], \tag{31}$$

where $V_{\rm ws}$ denotes volume of the Wiegner-Seitz cell. It is a contribution of the local orbital momentum to the conductivity. As has been already discussed[13,28] it is responsible for charge polarization in transport regime and that is why it can be called orbital polarization momentum. States with nonzero velocity along $\hat{y}$ direction contribute by the product $-xv_y$ and the Hall conductivity can be written as

$$\sigma_{xy}(E) = -\frac{e}{V_{\rm ws}}\sum_n [\vec{P}_n(E)]_z, \tag{32}$$

where the orbital polarization momentum $\vec{P}_n(E)$ reads

$$\frac{\vec{P}_n(E)}{V_{\rm ws}} \equiv -\frac{e}{8\pi^3}\int_{\rm BZ} \delta[E_n(\vec{k}) - E]\vec{r}_n(\vec{k}) \times \vec{v}_n(\vec{k})d^3k. \tag{33}$$

Here $\vec{r}_n(\vec{k})$ denotes the expectation value of the radius vector of the orbital n within the Wiegner-Seitz cell and integration is limited to the Brillouin-zone volume.

It can be easily shown that $\vec{P}_n(E)$ can be expressed in terms of the Berry-phase curvature. Since

$$\delta[E - E_n(\vec{k})] = -\frac{df_0[E_n(\vec{k})]}{dE_n(\vec{k})}, \tag{34}$$

where $f_0(E)$ denotes the zero-temperature Fermi-Dirac distribution, we get

$$\vec{P}_n(E) = -\frac{e}{h}\frac{V_{\rm ws}}{4\pi^2}\int_{\rm BZ} \{\vec{\nabla}_{\vec{k}} f_0[E_n(\vec{k})]\} \times \vec{r}_n(\vec{k})d^3k. \tag{35}$$

Integration by parts gives

$$\vec{P}_n(E) = \frac{e}{h}\frac{V_{\rm ws}}{4\pi^2}\int_{\rm BZ} f_0[E_n(\vec{k})][\vec{\nabla}_{\vec{k}} \times \vec{r}_n(\vec{k})]d^3k. \tag{36}$$

Using the expression derived in the Appendix for expectation values of the radius vector,

$$\vec{r}_n(\vec{k}) = -\int_{V_{\rm ws}} {\rm Im}[u^+_{n,\vec{k}}(\vec{r})\vec{\nabla}_{\vec{k}} u_{n,\vec{k}}(\vec{r})]d^3r, \tag{37}$$

we finally get

$$\frac{\vec{P}_n(E)}{V_{\rm ws}} = \frac{e}{h}\frac{1}{4\pi^2}\int_{\rm BZ} f_0[E_n(\vec{k})]\vec{\Omega}_n(\vec{k})d^3k, \tag{38}$$

where $\vec{\Omega}_n(\vec{k})$ is just the Berry-phase curvature,[14]

$$\vec{\Omega}_n(\vec{k}) = -{\rm Im}\int_{V_{\rm ws}} [\vec{\nabla}_{\vec{k}} u^+_{n,\vec{k}}(\vec{r})] \times [\vec{\nabla}_{\vec{k}} u_{n,\vec{k}}(\vec{r})]d^3r. \tag{39}$$

To conclude, the effect of Berry-phase curvatures is an alternative description to the presented effect of the orbital polarization moment, Eq. (33). It is equivalent to the Berry-phase correction to the orbital magnetization.[29]

VI. TIGHT-BINDING APPROACH AND SINGLE-SITE FLUCTUATIONS

The aim of this section is to present a simple model system allowing us to understand the main features of the anomalous Hall conductivity at zero external magnetic field. For the sake of simplicity the consideration will be limited to isotropic systems, like those of the cubic symmetry. A single-band model Hamiltonian will be considered of the following form:

$$H = \sum_l |l\rangle(E_a + \delta_l)\langle l| + \sum_{l,m}^{l\neq m} |l\rangle t_{lm}\langle m|, \tag{40}$$

where $|l\rangle$ and $|m\rangle$ are Wannier functions representing atomic-like orbitals associated with lattice sites $\vec{R}_l$ and $\vec{R}_m$, respectively. To model fluctuations, a variation δ_l of atomic-like orbital energies, E_a, will be considered, while hopping integrals t_{lm} are supposed to be fluctuation-independent quantities. This so-called diagonal disorder model covers variety of possible fluctuations representing, for example, alloy composition or local variation in the effective field $B_{\rm eff}$ which is supposed to have a fixed orientation independent on fluctuations. As concern thermal fluctuations they can be included by using deformation-potential approach[30] leading to Gaussian distribution of the fluctuation parameter δ_l. Note that this approach fails in the low temperature limit.

Instead of considering a specific form of the band dispersion for averaged Hamiltonian, $H_0 = \langle H\rangle_{\rm av}$, we shall assume it gives an elliptical density of states. In accord with Hubbard,[31] its energy dependence normalized per Wiegner-Seitz volume $V_{\rm ws}$ can be written as follows:

$$g(E) = 0, \quad |E - E_a| > w,$$

$$g(E) = \frac{2}{\pi w^2}\sqrt{w^2 - (E - E_a)^2}, \quad |E - E_a| \leq w, \tag{41}$$

where $2w$ denotes the bandwidth. The corresponding mean Fermi velocity reads

$$v_{\mathrm{F}} = \frac{w^2}{2\hbar}\left(\frac{\pi}{2}\right)^{2/3}\tilde{a}g(\mu), \tag{42}$$

where $\tilde{a} \equiv V_{\mathrm{ws}}^{1/3}$ just equals to the lattice constant for the simple cubic lattice. Note that this model system was already successfully applied to electron properties of substitutional alloys.[19] Under these simplifying assumptions the single-site orbital polarization moment defined by Eq. (33) becomes an energy-dependent quantity, given as

$$\vec{P}_l(E) = \vec{n}_a \tilde{a}^2 \frac{e}{h}\left(\frac{\pi}{2}\right)^{2/3}\frac{r_a(\delta_l)}{\tilde{a}}\left[1 - \left(\frac{E - E_a - \delta_l}{w}\right)^2\right], \tag{43}$$

where $r_a(\delta_l)$ denotes the average radius of the considered atomic-like orbital of the energy $E_a + \delta_l$ and $\vec{n}_a$ is the unit vector parallel to its orbital momentum. The only free model parameter in $\vec{P}_l(E)$, and consequently in anomalous Hall conductivity, Eq. (32), is the orbital radius. For $\tilde{a} \sim 3$ Å, and $r_a(0)/\tilde{a} \sim 0.3$, the corresponding anomalous Hall conductivity can reach values of several hundred of Ω^{-1} cm^{-1}, similar to those observed experimentally.

In real structures several overlapping energy bands contribute to the conductivity. Let us for simplicity consider two bands of the same width originated in atomic-like orbitals of energies $E_0 \pm \Delta E_a$. To model ferromagnetic state we assume that $\vec{B}_{\mathrm{eff}} = (0,0,B_{\mathrm{eff}})$, and that electron states belonging to different bands have opposite spin orientation along $\hat{z}$ direction, and opposite orientation of their local orbital moments. With rising energy of atomic orbitals their radius increases. Up to the lowest order in energy we get

$$\frac{r_a(E_a)}{\tilde{a}} = \frac{r_0}{\tilde{a}}\left(1 + \kappa\frac{E_a - E_0}{w}\right), \tag{44}$$

where r_0 denotes the radius for the orbital state of the energy E_0 and the parameter κ represents how the radius changes with the orbital energy.

Assuming that electron hopping between lattice sites is independent of their band origin, fluctuations of orbital energies $E_0 \pm \Delta E_a$ can be treated as independent. Ensemble averaging can thus be performed separately for each of the band contributions. Probability distribution of the fluctuation parameter δ depends on the fluctuation origin. Effect of different distribution functions has been tested. It has been found that the qualitative features of the conductivity tensor are not affected. For this reason the Lorentzian distribution allowing simple interpretation in terms of the electron lifetime is considered in the following treatment. It is given as

$$p(\delta,\Gamma) = \frac{1}{\pi}\frac{\Gamma}{\delta^2 + \Gamma^2}, \tag{45}$$

where the energy parameter Γ defines strength of the fluctuations. For the sake of simplicity so-called virtual-crystal approximation[19] is used to establish conductivity. In such a case the parameter Γ represents imaginary part of the self-energy Σ entering the effective Hamiltonian, Eq. (8), while the real part of the self-energy equals to zero. It also defines the electron lifetime, $\tau = \hbar/2\Gamma$.

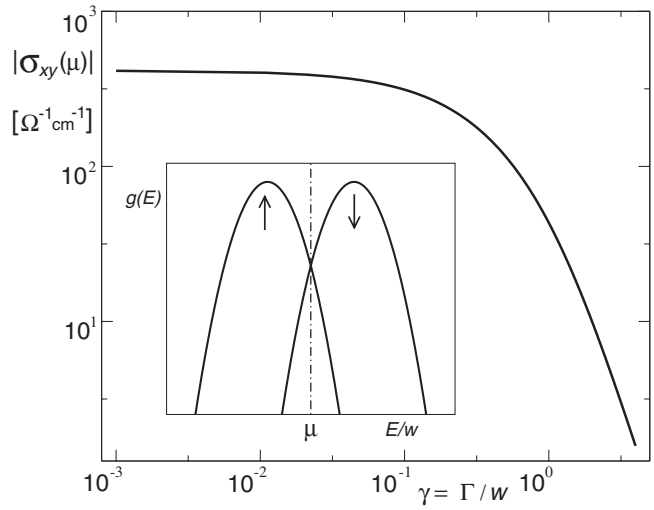

FIG. 1. Anomalous Hall conductivity for two-band model as a function of the fluctuation strength $\Gamma = \hbar/2\tau$. Used model parameters are specified in text. Inset shows corresponding density of states.

Substituting Eq. (43) into Eq. (32) for the anomalous Hall conductivity, and assuming there is one electron per lattice site, we get

$$\sigma_{xy}(\mu = E_0) = \frac{e^2}{\tilde{a}h}\left(\frac{\pi}{2}\right)^{2/3}\frac{r_0}{\tilde{a}} \times \int_{-1}^{+1}(1 - \xi^2)(1 + \kappa\xi) \times [p(\xi + \varepsilon, \gamma) - p(\xi - \varepsilon, \gamma)]d\xi, \tag{46}$$

where the half bandwidth w has been used as the energy unit, $\gamma \equiv \Gamma/w$, $\varepsilon \equiv \Delta E_a/w$. The resulting conductivity dependence on the fluctuation strength represented by the parameter $\gamma = \Gamma/w$ is shown on Fig. 1 for the following set of parameters: $\tilde{a} = 3$ Å, $r_a(0)/\tilde{a} = 0.3$, $\kappa = 1$, and $\varepsilon \equiv \Delta E_a/w = 0.6$.

The anomalous Hall conductivity dependence on the fluctuation strength Γ shows the same qualitative features as that found for multi-d-orbital tight-binding model developed by Kontani *et al.*[17] In the case of a weak disorder, $\Gamma/\Delta E_a \ll 1$, conductivity is nearly constant while for strong disorder, $\Gamma/\Delta E_a > 1$, it decreases with a power of the electron lifetime $\tau = \hbar/\Gamma$, which for the present example even slightly exceeds quadratic dependence. In comparison with the procedure used by Kontani *et al.* whose evaluation is based on the conductivity formula including only velocity operators, presented treatment based on local orbital polarization moments is much simpler and has a clear interpretation. Ferromagnetic state, necessary for appearance of anomalous Hall conductivity, can be characterized by average spin along magnetization axis which is supposed to be parallel with $\hat{z}$ direction. In the case of the considered two-band model it is assumed that each of them is fully spin polarized but in opposite directions, $s_z = \pm 1/2$. If there are no fluctuations the average spin per site $\langle s_z \rangle$ reaches a maximum value. Fluctuations of orbital energies can only lead to suppression of this value.

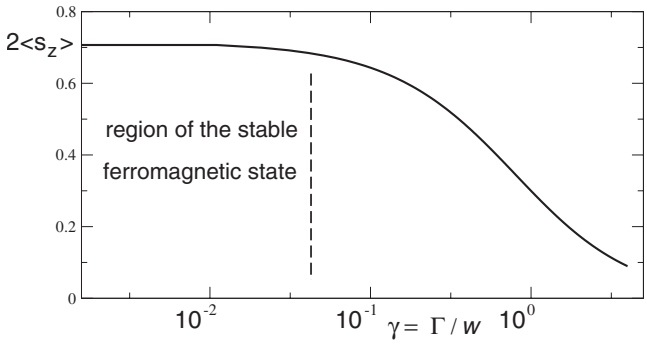

FIG. 2. Average spin $\langle s_z \rangle$ per site for two-band model as a function of the fluctuation strength $\Gamma = \hbar/2\tau$. Model parameters are the same as that used for the dependence presented in Fig. 1.

The dependence of $\langle s_z \rangle$ on the parameter Γ representing fluctuation strength is presented in Fig. 2 for the same set of parameters as that used for dependence presented in Fig. 1. It shows the same qualitative features as the dependence of the Hall conductivity on Γ. In the region where $\langle s_z \rangle$ is smaller than its maximum value the Hall conductivity depends on the fluctuation strength. It is the region in which fluctuations are strong enough to weaken ferromagnetic state.

Typical feature of the single-site model fluctuations is that vertex corrections vanish.[32] In the Eq. (21) defining the diagonal conductivity component σ_{xx} the ensemble averaging can thus be decoupled, i.e., $\langle GvG \rangle_{\rm av} \rightarrow \langle G \rangle_{\rm av} v \langle G \rangle_{\rm av}$. In this approximation relaxation time coincides with electron lifetime $\tau = \hbar/2\Gamma$. Using virtual-crystal approximation for the considered two-band model and probability distribution of fluctuations, Eq. (21), evaluation of σ_{xx} becomes trivial. In Fig. 3 obtained scaling of the Hall conductivity with σ_{xx} is shown. It reveals typical features observed experimentally.[1,16] Especially the case of the moderate disorder (good metal regime) for which $|\sigma_{xy}| \sim (\sigma_{xx})^0$ and that of the strong disorder (bad metal/hopping regime) for which $|\sigma_{xy}| \sim (\sigma_{xx})^{1.6}$.

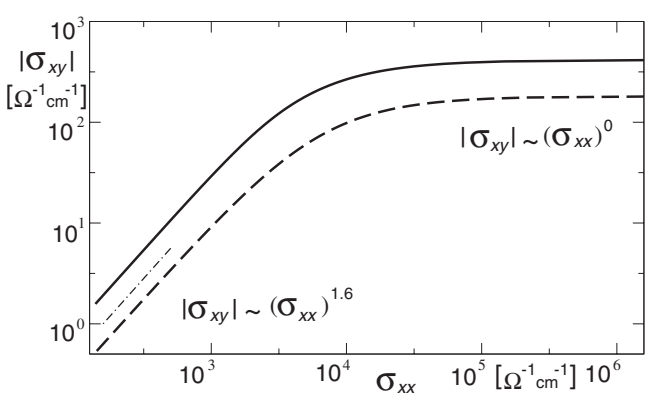

FIG. 3. Scaling of the Hall conductivity σ_{xy} with longitudinal conductivity σ_{xx}. Full line is given by the same model parameters as that used for the dependence presented in Fig. 1 while for dashed line the parameters κ and $\varepsilon \equiv \Delta E_a/w$ have been changed ($\kappa = 0.5$ and $\varepsilon = 0.4$). Dashed-dotted line shows the slope 1.6.

VII. CONCLUDING REMARKS

Transport theories of conductivity are traditionally formulated to give expressions containing velocity matrix elements only allowing standard analysis of the effect of different scattering events including vertex corrections. Their effect on anomalous Hall effect have been summarized in the review by Nagaosa *et al.*[1] Unfortunately the effect of the scattering on the Fermi-sea term, Eq. (25), has been ignored in their analysis. Derived alternative general form of the Hall conductivity formula given by Eq. (30) is compact, it does not separate Fermi-sea and Fermi-surface contributions. Required eigenfunctions of the coherent regions can be expressed in terms of matrix elements representing scattering of Bloch functions on impurities or other type of crystalline disorder. It is a challenge to perform such theoretical analysis which could be quite complicated because of the position operator entering the general formula. Nevertheless, for better understanding of the effect of different scattering processes such analysis is desirable.

For perfect Bloch electron system the derived alternative form of the Hall conductivity formula, Eq. (30), has been expressed in terms of the orbital polarizability momentum, Eqs. (32) and (33), which is a quantity determined by atomic-like orbitals. It is the part of the orbital magnetization of Fermi electrons given by the Berry-phase curvatures, Eq. (38). To estimate the effect of potential fluctuations the treatment was limited to those that can be modeled by the energy fluctuations of the local orbitals. Strictly speaking this single-site approach is applicable if coherent regions are of the dimension comparable with the size of atomic-like orbitals. In this case vertex corrections vanish[32] and the used model thus fails in the weak-scattering limit for which vertex corrections cannot be neglected. It is thus not applicable to high conductivity materials at low temperatures for which the most of different type of scattering events has been analyzed as reviewed by Nagaosa *et al.*[1] Especially skew scattering is excluded by the considered single-site model fluctuations with supposed fixed orientation of the effective field, $\vec{B}_{\rm eff}$. Also the effect of the interband side-jump scattering is fully ignored. The only considered intraband transitions are of the side-jump character since different Bloch states have different mass center positions induced by spin-orbit coupling.[13]

Despite of the model simplicity it correctly describes scaling of the anomalous Hall conductivity σ_{xy} with diagonal conductivity component σ_{xx} in the region covering the so-called good metal regime, $|\sigma_{xy}| \sim (\sigma_{xx})^0$, and the bad metal (hopping) regime, $|\sigma_{xy}| \sim (\sigma_{xx})^{1.6}$. In the good metal regime fluctuations only slightly affect the value of the Hall conductivity which is essentially determined by the value given by the limit of the perfect Bloch electron system. It is given by local polarizability moments which are equivalent to the Berry-phase correction to the orbital momentum, Eq. (38). In this case anomalous Hall effect is often called as intrinsic. The bad metal regime has been identified with the regime in which fluctuations become strong enough to weaken ferromagnetic state. In this regime the obtained scaling, $|\sigma_{xy}| \sim (\sigma_{xx})^{1.6}$, approximately corresponds to that experimentally observed on number of materials as reviewed by Nagaosa *et al.*[1]

To estimate anomalous Hall conductivity for a real material requires knowledge of local orbitals represented by Wannier functions and also the specific form of fluctuations relevant for the studied system. In particular, finite-temperature spin fluctuations are expected to be essential. It is a challenge to work out such a procedure based on the first-principles calculations. Recently developed numerical techniques allowing to establish Wannier functions giving the best tight-binding model parameters[33,34] together with the coherent-potential approximation[32] seem to be a proper way to establish anomalous Hall effect in real materials.

ACKNOWLEDGMENTS

The author acknowledges support from Grant Agency of the Czech Republic (Grant No. 202/08/0551) and the Institutional Research Plan No. AV0Z10100521. The author thanks Jan Kučera for useful comments and colleagues from Beijing University, Dingping Li for initializing this work, and Zhongshui Ma for fruitful discussions.

APPENDIX

Periodic part of Bloch functions can be expressed via Wannier functions $\phi_n(\vec{r}-\vec{R}_l)$ as follows:

$$u_{n,\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{l=1}^{N} e^{i\vec{k}(\vec{R}_l-\vec{r})}\phi_n(\vec{r}-\vec{R}_l), \tag{A1}$$

where by definition Wannier functions are orthonormal with respect to their mass-center position vector $\vec{R}_l$. The expectation value of the position vector $\vec{r}$ reads

$$\begin{aligned}
\vec{r}_n(\vec{k}) &= \langle n,\vec{k}|\vec{r}|n,\vec{k}\rangle = \frac{1}{2}\int [u^+_{n,\vec{k}}(\vec{r})\vec{r}u_{n,\vec{k}}(\vec{r}) + u_{n,\vec{k}}(\vec{r})\vec{r}u^+_{n,\vec{k}}(\vec{r})]dr^3 \\
&= \sum_{l=1}^{N}\int u^+_{n,\vec{k}}(\vec{r})\frac{\vec{r}-\vec{R}_l}{2\sqrt{N}}e^{-i\vec{k}(\vec{r}-\vec{R}_l)}\phi_n(\vec{r}-\vec{R}_l)d^3r \\
&\quad + \sum_{l=1}^{N}\int u_{n,\vec{k}}(\vec{r})\frac{\vec{r}-\vec{R}_l}{2\sqrt{N}}e^{i\vec{k}(\vec{r}-\vec{R}_l)}\phi^+_n(\vec{r}-\vec{R}_l)d^3r \\
&\quad + \sum_{l,l'=1}^{N}\frac{\vec{R}_l}{2N}\int e^{i\vec{k}(\vec{R}_l-\vec{R}_{l'})}\phi^+_n(\vec{r}-\vec{R}_{l'})\phi_n(\vec{r}-\vec{R}_l)d^3r \\
&\quad + \sum_{l,l'=1}^{N}\frac{\vec{R}_l}{2N}\int e^{i\vec{k}(\vec{R}_{l'}-\vec{R}_l)}\phi_n(\vec{r}-\vec{R}_{l'})\phi^+_n(\vec{r}-\vec{R}_l)d^3r \\
&= \frac{i}{2}\int [u^+_{n,\vec{k}}(\vec{r})\vec{\nabla}_{\vec{k}}u_{n,\vec{k}}(\vec{r}) - u_{n,\vec{k}}(\vec{r})\vec{\nabla}_{\vec{k}}u^+_{n,\vec{k}}(\vec{r})]d^3r + \frac{1}{N}\sum_{l=1}^{N}\vec{R}_l,
\end{aligned} \tag{A2}$$

where the last constant term represents the center of mass of the considered electron system. For states with $-\vec{k}$ the above relation gives

$$\vec{r}_n(-\vec{k}) = \mathrm{Im}\int u^+_{n,-\vec{k}}(\vec{r})\vec{\nabla}_{\vec{k}}u_{n,-\vec{k}}(\vec{r})d^3r + \frac{1}{N}\sum_{l=1}^{N}\vec{R}_l. \tag{A3}$$

Note that first term on the right-hand sides of Eqs. (A2) and (A3) are of the same absolute value but they have opposite sign.

In the summation over Fermi-surface states of the product $\vec{r}_n(\vec{k})\times\vec{v}_n(\vec{k})$ entering Eq. (33) the mass-center position of the electron system is cancelled out since $\vec{v}_n(\vec{k})=-\vec{v}_n(-\vec{k})$. The last term on the right-hand side of the above equation can thus be excluded from the consideration since it does not affect the final result.

[1] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys. **82**, 1539 (2010).
[2] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).
[3] M. Miyazawa, H. Kontani, and K. Yamada, J. Phys. Soc. Jpn. **68**, 1625 (1999).
[4] M. Onoda and N. Nogaosa, J. Phys. Soc. Jpn. **71**, 19 (2002).
[5] R. Shindou and N. Nagaosa, Phys. Rev. Lett. **87**, 116801 (2001).
[6] H. Kontani, T. Tanaka, D. S. Hirashima, K. Yamada, and J. Inoue, Phys. Rev. Lett. **100**, 096601 (2008).
[7] L. Berger, Phys. Rev. B **2**, 4559 (1970).
[8] J. Smit, Physica (Amsterdam) **24**, 39 (1958).
[9] J. M. Luttinger, Phys. Rev. **112**, 739 (1958).
[10] N. A. Sinitsyn, A. H. MacDonald, T. Jungwirth, V. K. Dugaev, and J. Sinova, Phys. Rev. B **75**, 045315 (2007).
[11] E. N. Adams and E. I. Blount, J. Phys. Chem. Solids **10**, 286 (1959).
[12] R. C. Fivaz, Phys. Rev. **183**, 586 (1969).
[13] P. Středa and T. Jonckheere, arXiv:1002.3212 (unpublished).
[14] G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).
[15] Y. Yao, L. Kleinman, A. H. MacDonald, J. Sinova, T. Jungwirth, D.-s. Wang, E. Wang, and Q. Niu, Phys. Rev. Lett. **92**, 037204 (2004).
[16] T. Miyasato, N. Abe, T. Fujii, A. Asamitsu, S. Onoda, Y. Onose, N. Nagaosa, and Y. Tokura, Phys. Rev. Lett. **99**, 086602 (2007).
[17] H. Kontani, T. Tanaka, and K. Yamada, Phys. Rev. B **75**, 184416 (2007).
[18] Time-dependent potential fluctuations are supposed to be slowly varying in time that electron states at given time are determined by the eigenvalue problem defined by the static potential just equal to that at given time.
[19] B. Velický, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. **175**, 747 (1968).
[20] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957); R. Kubo, A. Yokota, and S. Nakajima, *ibid.* **12**, 1203 (1957).
[21] In the derivation the terms containing the expression of the form $\delta(\eta-H)[G^{\pm}(\eta)]^{-1}=\epsilon(\eta-H\pm i\epsilon)^{-1}$ have been neglected since they are proportional to infinitesimal ε after any averaging procedure.

[22] A. Bastin, C. Lewinner, O. Betbeder-Matibet, and P. Nozieres, J. Phys. Chem. Solids **32**, 1811 (1971).
[23] D. A. Greenwood, Proc. Phys. Soc. London **71**, 585 (1958).
[24] L. Smrčka and P. Středa, J. Phys. C **10**, 2153 (1977).
[25] P. Středa, J. Phys. C **15**, L717 (1982); **15**, L1299 (1982).
[26] A. Crépieux and P. Bruno, Phys. Rev. B **64**, 094434 (2001).
[27] P. Středa, Phys. Status Solidi B **125**, 849 (1984).
[28] P. Středa, T. Jonckheere, and T. Martin, Phys. Rev. Lett. **100**, 146804 (2008).
[29] D. Xiao, Y. Yao, Z. Fang, and Q. Niu, Phys. Rev. Lett. **97**, 026603 (2006).
[30] A.-B. Chen, G. Weisz, and A. Sher, Phys. Rev. B **5**, 2897 (1972).
[31] J. Hubbard, Proc. R. Soc. London, Ser. A **281**, 401 (1964).
[32] B. Velický, Phys. Rev. **184**, 614 (1969).
[33] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997).
[34] X. Wang, J. R. Yates, I. Souza, and D. Vanderbilt, Phys. Rev. B **74**, 195118 (2006).