Středa-like formula in the spin Hall effect

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A generalized Středa formula is derived for the spin transport in spin-orbit coupled systems. As compared with the original Středa formula for charge transport, there is an extra contribution of the spin Hall conductance whenever the spin is not conserved. For recently studied systems with quantum spin Hall effect in which the z-component spin is conserved, this extra contribution vanishes and the quantized value of spin Hall conductivity can be reproduced in the present approach. However, as spin is not conserved in general, this extra contribution cannot be neglected, and the quantization is not exact.

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Intrinsic spin Hall effect (SHE) offers new possibility of designing semiconductor spintronic devices that do not require ferromagnetic elements or external magnetic fields. This effect has been theoretically predicted both in p-doped semiconductors with Luttinger type of spin-orbit (SO) coupling and in n-doped semiconductors with Rashba type of SO coupling.[1–3] In the hole-doped case,[1,2] the transverse spin current is generated by the Berry curvature correction to the group velocity of a Bloch wave packet,[4,5] which is similar to the case of the charge current in quantum Hall effect.[6] Later it is pointed out that the intrinsic SHE can even exist in band insulators with SO coupling, which are called spin Hall insulators.[7] These spin Hall insulators would allow spin currents to be generated without dissipation. This dissipationless character of the intrinsic SHE again finds analogy in the quantum Hall effect.

Pioneered by the work of Kane and Mele,[8] several specific single-particle Hamiltonians (graphene[8–10] and semiconductors[11–13]) giving rise to the quantum SHE (QSHE) have been proposed, in which the intrinsic spin Hall conductance can be quantized in units of $e/2\pi$. These models can be considered as multiple copies of the charge Hall effect with different values of the spin, arranged so that the time-reversal symmetry is unbroken and the spin current is nonzero in the presence of an applied electric field. The investigations on its stability with respect to interactions and disorders have just begun.[10,14,15]

Because there exists similarities between SHE and quantum Hall effect, one may wonder if some concepts used in quantum Hall effect can be generalized to SHE. It is well known that (integer) quantum Hall effect can be analyzed by the Středa formula.[6,16] Středa showed that, if the Fermi level falls within the energy gap, the Hall conductance can be given by the charge-density response to a magnetic field (from orbital, rather than Zeeman coupling). This formula has been used to calculate the conductance of an electron gas in the presence of an additional periodic potential.[17] It has also been generalized to three-dimensional systems.[18] Since the Středa formula is useful in quantum Hall effect, one may expect that similar formula for spin transport may be of some help in the study of SHE. Thus it is worthwhile to explore such a generalization.[19]

In the present work, we show explicitly that, similar to the well-known result of Středa,[16] there are two terms in the (static) spin Hall conductance σ_{sH}, one of which, σ^{I}_{sH}, is due to the electron states at the Fermi energy, and the other one, σ^{II}_{sH}, is formally related to the contribution of all occupied electron states below the Fermi energy. Since the proposed models for QSHE thus far are all band insulators, where the density of states at the Fermi level is zero, therefore $\sigma^{I}_{sH}=0$. Hence we are mainly interested in the contribution to QSHE from σ^{II}_{sH}. Furthermore, we show that σ^{II}_{sH} can be separated into a conserved part and a nonconserved part, in which the conserved part gives rise to a Středa-like contribution. That is, instead of directly calculating the spin-current response to an electric field, we can calculate the *spin-density* response to a magnetic field (again from orbital, rather than Zeeman coupling) to obtain the conserved part of σ^{II}_{sH}. However, another contribution to σ^{II}_{sH}, which comes from the nonconservation of spin, is not zero in general. We note that our derivation is model independent, and therefore it applies to any QSHE model. When this general formula is applied to the aforementioned specific models of QSHE with conserved electron spin, the quantized values of σ_{sH} can be easily reproduced. As the spin in a spin-orbit coupled system is not conserved in general, the non-Středa-like contribution in σ^{II}_{sH} cannot be neglected, and it can result in deviation from the quantized values, as shown in the numerical work of Ref. 10.

Using the linear response theory, the static spin Hall conductivity, for a z-component spin current flowing along the y direction under an electric field in the x direction, can be expressed as[20]

$$\sigma_{sH} = i\hbar\Omega \int d\varepsilon f(\varepsilon) \mathrm{Tr}\left[j^z_y \frac{dG^+(\varepsilon)}{d\varepsilon} j_x \delta(\varepsilon - H) - j^z_y \delta(\varepsilon - H) j_x \frac{dG^-(\varepsilon)}{d\varepsilon} \right], \tag{1}$$

where Ω is the volume of the system, $G^{\pm}(\varepsilon)=\lim_{\eta\to 0^+}(\varepsilon$

$-H\pm i\eta)^{-1}$ is the operator Green function of electrons described by the Hamiltonian H. $j_\mu(j_\mu^\alpha)$ is the charge (α-component spin) current density operator in μ direction. The trace goes over every eigenstate in the space of the Hamiltonian H. In Eq. (1), the delta function can be written in terms of Green functions, $\delta(\varepsilon-H)=-[G^+(\varepsilon)-G^-(\varepsilon)]/2\pi i$.

If we keep half of Eq. (1) and make an integration by parts on the second half, then σ_{sH} can be expressed as

$$\sigma_{sH}=\sigma_{sH}^I+\sigma_{sH}^{II}, \tag{2}$$

$$\sigma_{sH}^I=-\frac{i\hbar\Omega}{2}\int d\varepsilon\frac{\partial f(\varepsilon)}{\partial\varepsilon}\mathrm{Tr}[j_y^zG^+(\varepsilon)j_x\delta(\varepsilon-H)-j_y^z\delta(\varepsilon-H)j_xG^-(\varepsilon)], \tag{3}$$

$$\sigma_{sH}^{II}=\frac{\hbar\Omega}{4\pi}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\left[j_y^z\frac{dG^-(\varepsilon)}{d\varepsilon}j_xG^-(\varepsilon)-j_y^zG^-(\varepsilon)j_x\frac{dG^-(\varepsilon)}{d\varepsilon}-j_y^z\frac{dG^+(\varepsilon)}{d\varepsilon}j_xG^+(\varepsilon)+j_y^zG^+(\varepsilon)j_x\frac{dG^+(\varepsilon)}{d\varepsilon}\right]. \tag{4}$$

Here σ_{sH}^I stems from the contribution of electrons at the Fermi surface and σ_{sH}^{II} formally contains the contribution of all filled states below the Fermi energy. Note that at zero temperature, σ_{sH}^I is proportional to the density of states at the Fermi energy. Therefore, for band insulators, where the Fermi level lies within the band gap such that the density of states at the Fermi level is zero, $\sigma_{sH}^I=0$. Since we are interested in the band insulators with QSHE, we need only consider the contribution from σ_{sH}^{II}.

In order to simplify σ_{sH}^{II}, explicit expressions of j_x and j_y^z are needed. For systems with conserved (total) spin, the spin current can be uniquely defined (up to a term with zero divergence) through the equation of continuity. For systems with spin-orbit coupling, in which the spin is usually not conserved, the spin current cannot be uniquely defined.[21] In many experiments, the spin current can be measured as a spin flux in the external metal contacts, where there is no (or negligible) spin-orbit coupling. But one cannot infer the behavior of the spin current in the region of interest, which has spin-orbit coupling, through such a measurement.[21] Here the conventional definition for spin current is used, that is, $j_y^z\equiv\{v_y,s_z\}/2\Omega$.[22] The charge current density operator is $j_x=-ev_x/\Omega$, as usual.

Using the cyclic property of the trace operation and the relations

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

$$i\hbar v_\mu=[r_\mu,H]=-\left[r_\mu,\frac{1}{G^\pm(\varepsilon)}\right],$$

we find that the spin Hall conductance σ_{sH}^{II} can be separated into a "conserved" part $\sigma_{sH}^{II,(c)}$ and a "nonconserved" part $\sigma_{sH}^{II,(n)}$,

$$\sigma_{sH}^{II}=\sigma_{sH}^{II,(c)}+\sigma_{sH}^{II,(n)}, \tag{5}$$

$$\sigma_{sH}^{II,(c)}=\frac{e}{4\pi i\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\{s_zG^+(xv_y-yv_x)G^+-s_zG^-(xv_y-yv_x)G^-\}, \tag{6}$$

$$\begin{aligned}\sigma_{sH}^{II,(n)}=&-\frac{i\hbar^2e}{4\pi\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\{\dot{s}_z[(G^+)^2v_xG^+v_yG^++G^+v_yG^+v_x(G^+)^2-\mathrm{H.c.}]\}\\&-\frac{\hbar e}{8\pi\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}\{\dot{s}_z[G^+[y,v_x](G^+)^2+(G^+)^2[y,v_x]G^++\mathrm{H.c.}]\}.\end{aligned} \tag{7}$$

Here we call $\sigma_{sH}^{II,(n)}$ as the nonconserved part because it contains terms with $\dot{s}_z\equiv[s_z,H]/i\hbar$ and therefore vanishes if s_z is conserved. The nonconserved part can be simplified under certain situation. For example, if the momentum of the orbit couples with the spin linearly, such as the Rashba-Dresselhaus SO coupling in two-dimensional electron gas, then the commutator $[y,v_x]=0$, and the second line in Eq. (7) vanishes.

By employing the identity[23]

$$\frac{\partial}{\partial B}\mathrm{Tr}\{s_z\delta(\varepsilon-H)\}=\frac{-e}{4\pi i}\mathrm{Tr}\{s_zG^+(xv_y-yv_x)G^+-s_zG^-(xv_y-yv_x)G^-\}, \tag{8}$$

the conserved part $\sigma_{sH}^{II,(c)}$ can be rewritten as a generalized Středa formula for SHE,

$$\sigma_{sH}^{II,(c)}=-\left.\frac{\partial S_z}{\partial B}\right|_{\mu,T}, \tag{9}$$

where B is the magnitude of a uniform external magnetic field in the z direction, μ is the chemical potential, T is the temperature, and S_z is the z-component spin density,

$$S_z=\frac{1}{\Omega}\int d\varepsilon f(\varepsilon)\mathrm{Tr}[s_z\delta(\varepsilon-H)]. \tag{10}$$

Equation (9) shows the relation between the spin Hall conductivity and the derivative of the z-component spin density with respect to the perpendicular magnetic field B. Equations (3), (7), and (9), are the main results of this paper.

Some comments are in order. Contrary to the case of the original Středa formula for charge transport,[16] there always exists an extra contribution for σ_{sH}^{II} besides the Středa-like one as long as the spin is not conserved. Moreover, following the same reasoning of the present derivation, it is obvious that, for a current carrying some *conserved* quantity, there will always be a corresponding Středa-like formula. For example, when the total angular momentum J_z consisting of both spin and orbit angular momenta is conserved, the Hall conductivity for the *total-angular-momentum current* can be calculated through the *total-angular-momentum density* response to a magnetic field. That is, a Středa-like formula in which s_z is replaced by J_z can be derived.

In the following, we illustrate the application of the present approach to two of the aforementioned QSHE models. As mentioned earlier, since the proposed models for QSHE thus far are all band insulators, including this two models, we need to consider only the contribution from σ_{sH}^{II}. In the first example, Bernevig and Zhang considered the conduction electron in a semiconductor with zinc-blende structure, such as GaAs.[11] In this type of materials, it is possible to generate a velocity-dependent force on the electron by applying a shear strain gradient. The electron spin is coupled to the velocity and the strain in such a way that mimics the usual spin-orbit coupling. By carefully choosing the strain configuration, in combination with a parabolic confinement potential, they are able to generate an effective (uniform) magnetic field. It is shown in Ref. 11 that, because of a linear strain gradient, there exist opposite effective orbital magnetic fields $\pm B_{\text{eff}}$ acting on spin $\uparrow$ and $\downarrow$ electrons. Thus degenerate quantum Landau levels are created and then σ_{sH} becomes quantized in units of $e/2\pi$.

This result can be understood as follows. Even though the intrinsic SO coupling is present, s_z remains conserved in this case. Therefore, the nonconserved part $\sigma_{sH}^{II,(n)}=0$ and the spin Hall conductance comes merely from the Středa-like one [Eq. (9)], which is the spin-density response to an infinitesimal external magnetic field δB in the z direction (at a fixed chemical potential). When a weak external magnetic field δB ($\ll B_{\text{eff}}$) is turned on, the total effective fields acting on spin $\uparrow$ and $\downarrow$ electrons will become $\pm B_{\text{eff}}+\delta B$ such that the degeneracies per unit area of the corresponding Landau levels become $(B_{\text{eff}}\pm\delta B)e/h$. Therefore, for a fixed chemical potential lying within the gap between the Nth and the $(N+1)$th Landau levels, the number density of electrons with spin $\uparrow$ and $\downarrow$ becomes $n_{\uparrow/\downarrow}=N(B_{\text{eff}}\pm\delta B)e/h$ and the induced spin density becomes $\delta S_z=(\hbar/2)(n_\uparrow-n_\downarrow)=(Ne/2\pi)\delta B$. Thus, using Eq. (9), $\sigma_{sH}=\sigma_{sH}^{II,(c)}=Ne/2\pi$ can be obtained.

As the next application of our formula, we consider the tight-binding model of graphene proposed by Kane and Mele.[8] They considered a generalization of Haldane's graphene model that exhibits quantum Hall effect in the absence of a uniform magnetic field.[24] In the original model, the electron is spinless and one has to consider second-neighbor hopping, in combination with a periodic magnetic field that has zero mean flux per unit cell, to open gaps at the corners of the Brillouin zone. In Ref. 8, by including electron spin with a time-reversal invariant SO interaction, one does not require a periodic magnetic field to produce similar gaps that reveal the topology of the electron bands in such a material.

In the *absence* of the Rashba SO coupling term, it is shown that this model can give rise to QSHE with a quantized spin Hall conductivity $\sigma_{sH}=e/2\pi$. This result can also be obtained by the present approach. For this model of graphene *without* the Rashba SO coupling, spin s_z is conserved. Again, $\sigma_{sH}^{II,(n)}=0$ and the spin Hall conductance comes from the Středa-like one [Eq. (9)] only. As mentioned in Ref. 8, each independent subsystem of spin direction ($\uparrow$ or $\downarrow$) is equivalent to Haldane's model for spinless electrons,[24] where the mass gaps at different corners (say, the K and the K' points) of the hexagonal Brillouin zone of a honeycomb lattice of carbon atoms have different signs. Therefore, as shown by Haldane, at zero temperature and with a fixed chemical potential, the application of a weak external magnetic field δB will induce an extra *field-dependent* number density of electrons $\Delta n_{\uparrow/\downarrow}=\text{sgn}(m_{\uparrow/\downarrow})(e/h)\delta B$, where $m_{\uparrow/\downarrow}$ denotes the mass gap for each spin component at a particular corner (say, the K point) of the hexagonal Brillouin zone.[24] Since $m_\downarrow=-m_\uparrow$ for the QSHE model proposed in Ref. 8, the induced spin density by applying a weak external magnetic field δB becomes $\delta S_z=(\hbar/2)(2e/h)\delta B=(e/2\pi)\delta B$. Thus, using Eq. (9), $\sigma_{sH}=\sigma_{sH}^{II,(c)}=e/2\pi$ can again be reached.

In generic cases, spin is not conserved in the presence of a SO interaction and therefore spin current is not well defined. As done in Ref. 2, one can separate the spin operator s_z into a conserved part $s_z^{(c)}$ and a nonconserved part $s_z^{(n)}$: $s_z=s_z^{(c)}+s_z^{(n)}$, where the conserved part $s_z^{(c)}$ consists of only intraband matrix elements of the spin. Thus a conserved spin current can be defined by substituting the conserved part $s_z^{(c)}$ into the conventional expression of spin current. By employing this definition of spin current, it can be shown that the nonconserved part $\sigma_{sH}^{II,(n)}$ vanishes and the conserved part $\sigma_{sH}^{II,(c)}$ again obeys the Středa-like formula, Eq. (9), in which the spin operator s_z is replaced by $s_z^{(c)}$. In Ref. 25, another definition of the spin current is proposed which includes the torque dipole density. If we use this definition in the derivation for σ_{sH}^{II}, the Středa-like formula Eq. (9) for the conserved part $\sigma_{sH}^{II,(c)}$ remains valid, and the nonconserved part $\sigma_{sH}^{II,(n)}$ remains nonzero and has different expression from Eq. (7).

In conclusion, a generalized Středa formula is derived for spin transport, which relates the spin Hall conductivity with the spin density response to an external magnetic field when the energy bands are filled. For systems in which the spins are not conserved, there is an additional contribution to the spin-density response term. The present approach is most convenient for the recently proposed QSHE systems with conserved spin and filled energy bands. We demonstrate that their results on the quantized spin Hall conductivity can be reproduced with great ease. Since the original Středa formula has been useful in analyzing the quantum Hall effect in the presence a periodic potential if the Fermi level lies within a miniband gap,[17,18] we expect the generalized Středa formula will be helpful for the spin transport under the same situation.[26] However, unlike the charge Hall effect, there is generically no conserved spin density in the presence of spin-orbit coupling. This could make the applicable range of the Středa-like formula more restricted.

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