Off-Fermi surface cancellation effects in spin-Hall conductivity of a two-dimensional Rashba electron gas

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We calculate the spin-Hall conductivity of a disordered two-dimensional Rashba electron gas within the self-consistent Born approximation and for arbitrary values of the electron density, parametrized by the ratio $E_F/E_0$, where $E_F$ is the Fermi level and $E_0$ is the spin-orbit energy. We confirm earlier results indicating that in the limit $E_F/E_0 \gg 1$ the vertex corrections suppress the spin-Hall conductivity. However, for sufficiently low electron density such that $E_F \lesssim E_0$, we find that the vertex corrections no longer cancel the contribution arising from the Fermi surface, and they cannot therefore suppress the spin current. This is instead achieved by contributions away from the Fermi surface, disregarded in earlier studies, which become large when $E_F \lesssim E_0$.

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The spin-Hall effect, i.e., the generation of a spin polarized current transverse to the direction of an applied external electric field, has recently raised considerable interest in view of its possible application in spintronics. Alongside the extrinsic spin-Hall effect generated by the spin-orbit (SO) coupling to impurities and defects, much theoretical effort has been devoted to the intrinsic spin-Hall effect arising from the one-particle band structure of spin-orbit coupled systems.\textsuperscript{1,2,3} The initial claim that for a two-dimensional (2D) electron gas subject to the Rashba SO coupling the intrinsic spin-Hall conductivity, $\sigma_{\text{SH}}$, is a universal constant ($\sigma_{\text{SH}} = |e|/8\pi m^2$) which reduce $\sigma_{\text{SH}}$ to zero\textsuperscript{4,5,6,7,8} at the same time, however, for other models of SO coupling, like, for example, the three-dimensional (3D) Dresselhaus model\textsuperscript{9} the Luttinger model for valence band holes\textsuperscript{10,11} or generalized Rashba models taking into account non linear momentum dependences of the SO interaction\textsuperscript{12,13,14,15} or a non-quadratic unperturbed band spectrum\textsuperscript{16} $\sigma_{\text{SH}}$ has been found to be robust against non-magnetic impurity scatterings, suggesting that the vanishing of $\sigma_{\text{SH}}$ is a peculiar feature of the linear Rashba model. This is also supported by rather general arguments which do not rely on the specific scattering process\textsuperscript{12,13,14,15}.

Within the linear response theory, the vanishing of $\sigma_{\text{SH}}$ in the Rashba model has been ascribed to a cancellation effect of the spin-dependent part of the ladder current vertex in the Born approximation for impurity scattering\textsuperscript{4,5,6,7,8}. This cancellation basically follows from the fact that, as long as the Fermi energy $E_F$ is much larger than the spin-orbit energy $E_0$, the factor $\tau^{-1}$ associated with the current vertex (where $\tau$ is the electron life-time due to impurities) is balanced by the factor $\tau$ arising from the product of two Greens functions appearing in the current vertex kernel. However, similarly to what happens for other properties (e.g., the conductivity in impure metals), such kinds of balance effects are usually peculiar to the assumption that $E_F$ is the largest energy scale of the problem, and one may wonder if the cancellation mechanism based on the vertex function described in Refs.\textsuperscript{4,5,6,7,8} is still valid when $E_F$ is comparable with $E_0$. The clarification of this issue is important not only to assess the role of vertex corrections in a general context, but it is also quite crucial in view of the recent progress made in fabricating systems with large SO couplings for which the $E_F \gg E_0$ approximation may not be appropriate. Examples of such large SO systems are, among others, HgTe quantum wells\textsuperscript{16} the surface states of metals and semimetals\textsuperscript{17,18} and even the heavy Fermion superconductor CePt$_3$Si\textsuperscript{19}. However the most striking example is provided by bismuth/silver(111) surface alloys displaying quadratic unperturbed bands split by a Rashba energy of about $E_0 = 220$ meV\textsuperscript{20}. In this system the Fermi energy can be tuned by doping with lead atoms in such a way that $E_F$ may be larger or lower than $E_0$\textsuperscript{20,21}.

In this paper we investigate the spin-Hall conductivity in the Born approximation of impurity scattering and for arbitrary values of $E_F/E_0$. We find that, apart from the high density limit $E_F/E_0 \rightarrow \infty$, the spin-dependent part of the vertex function is generally not zero, and increases as $E_F/E_0$ decreases, eventually reaching unity as $E_F \rightarrow 0$. In this situation, the spin-Hall conductivity $\sigma_{\text{SH}}$ would be nonzero if calculated along the lines of Refs.\textsuperscript{4,5,6,7,8}, in contradiction with the general arguments of Refs.\textsuperscript{4,5,6,7,8}. We resolve this inconsistency by showing that $\sigma_{\text{SH}}$ is actually canceled by the contributions away from the Fermi surface, which have magnitude equal to those on the Fermi surface, but opposite in sign.

We consider a 2D Rashba electron gas whose Hamiltonian is

$$H = \frac{\hbar^2 k^2}{2m} + \gamma (k_x \sigma_y - k_y \sigma_x),$$

(1)
where $m$ is the electron mass, $k$ is the electron wave-number, and $\gamma$ is the SO coupling. The corresponding electron dispersion consists of two branches $E_s^k = h^2(k^2 + sk_0)^2/2m$ where $s = \pm 1$ is the helicity number and $k_0 = m\gamma/h^2$. In the following, we parametrize the SO interaction by the Rashba energy $E_0 = h^2k_0^2/2m$ that, for a clean system, corresponds to the minimum inter-band excitation energy for an electron at the bottom of the lower ($s = -1$) band. For simplicity, we consider a short-ranged impurity potential of the form $V(r) = V_{\text{imp}}\sum_i \delta(r - R_i)$, where the summation is performed over random positions $R_i$ of the impurity scatterers with density $n_i$. The corresponding electron Green’s function is a $2 \times 2$ matrix in the spin space,

$$G(k, i\omega_n) = \frac{1}{2} \sum_{s=\pm} \left[ 1 + s(\hat{k}_x \sigma_y - \hat{k}_y \sigma_x) \right] G_s(k, i\omega_n), \quad (2)$$

where $G_s(k, i\omega_n)^{-1} = i\omega_n - E_s^k + \mu - \Sigma(i\omega_n)$ is the electron propagator in the helicity basis, $\mu$ is the chemical potential, $\omega_n = (2n + 1)\pi T$ is the Matsubara frequency where $T$ is the temperature, and $\Sigma(i\omega_n)$ is the impurity self-energy in the self-consistent Born approximation,

$$\Sigma(i\omega_n) = \frac{1}{2\pi T N_0} \int \frac{dk}{(2\pi)^2} G(k, i\omega_n)$$

$$= \frac{1}{4\pi T N_0} \sum_{s=\pm} \int \frac{dk}{2\pi} k G_s(k, i\omega_n), \quad (3)$$

where $\tau^{-1} = 2\pi n_i V_{\text{imp}}^2 N_0 / \hbar$ is the scattering rate for a 2D electron gas with zero SO interaction and density of states $N_0 = m/2\pi\hbar^2$ per spin direction. The spin-Hall conductivity is obtained from

$$\sigma_{\text{SH}} = -\lim_{\omega \to 0} \frac{\text{Im}K_{sc}(\omega + i\delta)}{\omega} \quad (4)$$

where $K_{sc}$ is the spin-current–charge-current correlation function given by

$$K_{sc}(i\omega_m) = \frac{T}{\pi} \sum_n \int \frac{dk}{(2\pi)^2} \text{Tr} \left[ j^y_s(k) G(k, i\omega_n + i\omega_m) \right],$$

$$J^y_s(k, i\omega_n + i\omega_m) = \frac{1}{2\pi T N_0} \sum_{s=\pm} \int \frac{dk'}{(2\pi)^2} \left[ G(k', i\omega_l) J^y_s(k', i\omega_l, i\omega_n) G(k', i\omega_n) \right]. \quad (5)$$

Here $j^y_s(k) = \{ S_z, v_y(k) \} / 2 = h^2k_y \sigma_z / 2m$ is the current operator in the $y$ direction for spins polarized along $z$ and $J^y_s$ is the vertex function for charge current along the $x$ direction. In the Born approximation for impurity scattering, $J^y_s$ satisfies the following ladder equation:

$$J^y_s(k, i\omega_l, i\omega_n) = j^y_s(k)$$

$$+ \frac{1}{2\pi T N_0} \int \frac{dk'}{(2\pi)^2} G(k', i\omega_l) J^y_s(k', i\omega_l, i\omega_n) G(k', i\omega_n), \quad (6)$$

where $j^y_s(k) = e\nu_e(k) = e\hbar k_x / m + e\gamma \sigma_y / \hbar$ is the bare charge current. Equation (6) can be rewritten as

$$J^y_s(k, i\omega_l, i\omega_n) = e\hbar k_x / m + e\gamma \sigma_y / \hbar \right \} \hbar \gamma$$

represents the SO corrections to the charge current function. By using Eq. (2) and by taking advantage of the momentum independence of $\Sigma$, the correlation function $K_{sc}$ reduces to

$$K_{sc}(i\omega_m) = \frac{i\hbar^2}{4m} \sum_n \Gamma_y(i\omega_n + i\omega_m, i\omega_n)$$

$$\times B_1(i\omega_n + i\omega_m, i\omega_n)$$

$$= \frac{\hbar^2}{4m} \sum_n B(i\omega_n + i\omega_m, i\omega_n) \quad (7)$$

where $\Gamma_y$ is the component of $\Gamma$ proportional to $\sigma_y$, $\gamma_y = \text{Tr}(\sigma_y \Gamma)$, and becomes

$$\gamma_y(i\omega_l, i\omega_n) = \frac{8\pi T N_0 + \frac{1}{k_0} B_2(i\omega_l, i\omega_n)}{8\pi T N_0 - B_3(i\omega_l, i\omega_n)} \quad (8)$$

In Eqs. (7) and (8) the function $B_1$, $B_2$, and $B_3$ are

$$B_1(i\omega_l, i\omega_n) = \int \frac{dk}{2\pi} k^2 \sum_s G_{-s}(k, i\omega_l) G_s(k, i\omega_n), \quad (9)$$

$$B_2(i\omega_l, i\omega_n) = \int \frac{dk}{2\pi} k^2 \sum_s G_s(k, i\omega_l) G_s(k, i\omega_n), \quad (10)$$

$$B_3(i\omega_l, i\omega_n) = \int \frac{dk}{2\pi} k \sum_{s,s'} G_s(k, i\omega_l) G_{s'}(k, i\omega_n). \quad (11)$$

At this point, the analytical continuation to the real axis, $i\omega_m \to \omega + i\delta$, can be performed by following the usual steps leading to

$$T \sum_n K(i\omega_n + i\omega_m, i\omega_n)$$

$$\to - \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} [f(\epsilon + \omega) - f(\epsilon)] \text{Im}K(\epsilon + \omega + i\delta, \epsilon - i\delta) \quad (12)$$

where $f(x) = 1 / [\exp(x/T) + 1]$ is the Fermi distribution function. When the spin-Hall conductivity is evaluated via Eq. (11), it is clear that the resulting $\sigma_{\text{SH}}$ will be given by the sum of two contributions, $\sigma_{\text{SH}}^{RA}$ and $\sigma_{\text{SH}}^{RH}$, respectively, defined as the first and second line in the right-hand side of Eq. (12), and characterized by different combinations of retarded (R) and advanced (A) Green’s functions (see below). The first term, $\sigma_{\text{SH}}^{RA}$, contains in the limit $\omega \to 0$ the term $df(\epsilon)/d\epsilon$ which, for $T = 0$, restricts all quasiparticle contributions to the Fermi surface. The second term instead has an integral containing $f(\epsilon)$, allowing therefore for processes away from the Fermi surface. In Refs. [4, 6, 7, 8], this term has been disregarded because in the large $E_F$ limit it scales as $E_0/(\tau E_F)$ and the spin-Hall conductivity has been approximated by the $\sigma_{\text{SH}}^{RA}$ contribution alone, which at zero temperature re-
\[ \sigma_{sh}^{RA} = -\frac{\hbar^2 \gamma}{8\pi m} \Gamma_y^{RA} \int \frac{dk}{2\pi} k^2 \sum_s G^R_s(k,0)G^A_s(k,0). \]  

(13)

Here \( G^R(A) \) is the retarded (advanced) Green’s function and \( \Gamma_y^{RA} = \Gamma_y (0 + i\delta, 0 - i\delta) \) is the ladder vertex function calculated at \( i\omega_n = i\delta \) and \( i\omega_n = -i\delta \). By assuming that the SO energy \( E_0 \) is negligible with respect to \( E_F \), then the self-energy \( \Sigma \) can be approximated as \( \Sigma^R(\omega) = -i/2\pi \Sigma \) and the bubble term \( \Sigma_B \) defined in Eq. (10) reduces to \( \Sigma_B (i\delta, -i\delta) = -8\pi N_0 k_0 \), which by using Eq. (5), leads to \( \Gamma_y^{RA} = 0 \). This is the vertex cancellation mechanism pointed out in Refs. [15,17].

We reexamine now Eq. (13) by relaxing the hypothesis \( E_F \gg E_0 \). For practical purposes, we introduce an upper momentum cut-off \( k_c \), such that all the relevant momentum and energy scales are much smaller than the corresponding cut-off quantities, namely \( k_0, k_F \ll k_c, E_F, E_0 \). After the analytical continuation, the integration over momenta in Eq. (13) can be performed analytically and the real axis self-energy is evaluated numerically by iteration. The obtained \( \Sigma \) is then substituted into \( \Gamma_y^{RA} \) and \( \sigma_{sh}^{RA} \), Eq. (13), whose momentum integration allows for an analytical evaluation due to the momentum independence of \( \Sigma \). To explore the effect of varying \( E_F \) on the spin-Hall conductivity, we have first evaluated the Green’s functions at fixed number electron density \( n \), where \( n = 2 \) \((n = 0)\) means that all states below the cut-off energy \( E_c \) are filled (empty), and subsequently the corresponding \( E_F \) for a given \( n \) has been extracted from

\[ n = \frac{1}{2E_c} \int_{-\infty}^{\infty} d\omega f(\omega) \sum_s N_s(\omega) / N_0, \]

(14)

where \( N_s(\omega) = -(1/\pi) \int dk / 2\pi k \Im G^R_s(k,\omega) \) is the density of states for the interacting system and \( f(\omega) = \theta(-\omega) \) at zero temperature.

In Fig. 1(a) we report the SO vertex function \( \Gamma_y^{RA} \) as a function of \( E_F \tau \) and for several values of the SO energy \( E_0 \) ranging from \( E_0 \tau = 0.8 \) up to \( E_0 \tau = 4 \) (from bottom to top). The coupling to the impurity potential has been set equal to \( E_c \tau = 80 \) in all cases. The corresponding values of the number electron density \( n \) as a function of \( E_F \) of the interacting system are plotted in the inset of Fig. 1(a). For \( E_F \tau \simeq 10 \), the Fermi energy \( E_F \) is sufficiently large compared to \( E_0 \) and \( \Gamma_y^{RA} \) is negligibly small, confirming the results reported in Refs. [15,17]. However, as \( E_F \tau \) is decreased, \( \Gamma_y^{RA} \) increases monotonically up to \( \Gamma_y^{RA} \simeq 1 \) for \( E_F/E_0 \simeq 0 \). In these circumstances, therefore, the vertex cancellation mechanism is no longer active, and the corresponding spin-Hall conductivity \( \sigma_{sh}^{RA} \) is expected to be non-zero. This is indeed shown in Fig. 1(b) where \( \sigma_{sh}^{RA}, \) Eq. (13), is plotted in units of \( |e|/8\pi \) as a function of \( E_F \tau \). The nonmonotonic behavior of \( \sigma_{sh}^{RA} \) is due to the competition between the increase of \( \Gamma_y^{RA} \) shown in Fig. 1(a) and the decrease of the integral appearing in Eq. (13) as \( E_F \rightarrow 0 \).

A non-vanishing spin-Hall conductivity in an impure 2D Rashba electron gas is at odds with the general arguments of Refs. [15,17] where \( \sigma_{sh} \) has been shown to be zero for any spin-conserving momentum scattering, independently of the ratio \( E_0/E_F \). However, as already pointed out above, the physical spin-Hall response is not entirely defined by Eq. (13), but should also include the contributions away from the Fermi surface given by the second term in the right-hand side of Eq. (12). Hence

\[ \sigma_{sh} = \sigma_{sh}^{RA} + \sigma_{sh}^{RR}, \]

where

\[ \sigma_{sh}^{RR} = \frac{\hbar^2 \gamma}{4\pi m} \Im \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \Gamma_y^{RR}(\epsilon) \times \int \frac{dk}{2\pi} k^2 \sum_s \frac{dG^R_s(k,\epsilon)}{d\epsilon} G^R_s(k,\epsilon), \]

(15)

and \( \Gamma_y^{RR}(\epsilon) = \Gamma_y (\epsilon + i\delta, \epsilon + i\delta) \).

Our numerical calculations of \( \sigma_{sh}^{RR} \), Eq. (15), are plotted in Fig. 1(b) (dashed lines) together with the corresponding \( \sigma_{sh}^{RA} \) results already plotted in Fig. 1(a). For all \( E_F/E_0 \) values, \( \sigma_{sh}^{RR} \) has the same magnitude of \( \sigma_{sh}^{RA} \) but...
FIG. 2: The different contributions to the spin-Hall conductivity for the same parameters of Fig. 1: $\sigma^{RA}_{\text{sh}}$ (solid lines), $\sigma^{RR}_{\text{sh}}$ (dashed lines), and the physical spin-Hall conductivity $\sigma_{\text{sh}} = \sigma^{RA}_{\text{sh}} + \sigma^{RR}_{\text{sh}}$ (gray lines). All conductivities are given in units of $|e|/8\pi$.

with opposite sign, so that the resulting physical spin-Hall conductivity, $\sigma_{\text{sh}} = \sigma^{RA}_{\text{sh}} + \sigma^{RR}_{\text{sh}}$ (gray lines) reduces to zero within the accuracy of our numerical calculations.

The results plotted in Fig. 2 clearly demonstrate that, generally, a correct evaluation of the spin-Hall conductivity must take into account the contributions away from the Fermi surface, resolving therefore the concerns expressed in Ref. 11 about an only-on-Fermi-surface cancellation mechanism. However, on this point, a few remarks should be brought to attention. First, the cancellation between $\sigma^{RA}_{\text{sh}}$ and $\sigma^{RR}_{\text{sh}}$ suggests that, by suitable mathematical transformations, the (nominal) off-Fermi surface contribution 15 may be expressed as $-\sigma^{RA}_{\text{sh}}$, resulting in a cancellation mechanism that is, after all, a Fermi surface property. However, we have been unable to find such a transformation. A second possibility is that $\sigma^{RA}_{\text{sh}}$ is, generally, a genuine off-Fermi surface quantity, but that, accidentally, for the model Hamiltonian of Eq. (1), such a term is quantitatively equal to $-\sigma^{RA}_{\text{sh}}$. In this case, any variation from the linear Rashba model of 11 would result in $\sigma^{RA}_{\text{sh}}$ and $\sigma^{RR}_{\text{sh}}$ terms which do not mutually cancel, leading to a nonzero spin-Hall conductivity. In this respect, one should note that, in fact, the general arguments of Refs. 11-13 about the vanishing of $\sigma_{\text{sh}}$ apply only for model Hamiltonians of the type 11.

Before concluding, it is worth stressing that the results presented in this work could be relevant also for systems described by non-linear Rashba or 3D Dresselhaus SO couplings, or by non-quadratic unperturbed electronic band structures. It is known that for such systems, the spin-Hall conductivity in the presence of momentum scattering is non-zero also for $E_F/E_0 \to \infty$ because the SO vertex does not vanish. 9,10,11,12,13,14 Our results suggest, however, that even in this case, for finite $E_F/E_0$, a quantitatively reliable calculation of $\sigma_{\text{sh}}$ should take into account also the off-Fermi surface contributions. This could be for example the case of the system studied in Ref. 15 where $E_F$ is of the same order as $E_0$ and the unperturbed band spectrum is clearly non-quadratic.

In conclusion, we have calculated the spin-Hall conductivity $\sigma_{\text{sh}}$ for a 2D electron gas subjected to the linear Rashba SO coupling in the Born approximation for impurity scattering. We have shown that, apart from the $E_F \to \infty$ limit, the spin-dependent part of the vertex function is nonzero and increases as $E_F \to 0$, leading to nonzero Fermi surface contribution $\sigma^{RA}_{\text{sh}}$ to the spin-Hall conductivity. We have demonstrated that the physical spin-Hall conductivity $\sigma_{\text{sh}}$ actually includes also contributions away from the Fermi surface, $\sigma^{RR}_{\text{sh}}$, which are as large as those on the Fermi surface, but of opposite sign, leading to a vanishing $\sigma_{\text{sh}}$ for arbitrary values of $E_F/E_0$.

We expect that, given the arguments of Refs. 11-15, the mutual cancellation of $\sigma^{RA}_{\text{sh}}$ and $\sigma^{RR}_{\text{sh}}$ for $E_F < \infty$ holds true also beyond the self-consistent Born approximation employed here.

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