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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,[1] 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.[2,3] The initial claim that for a two-dimensional (2D) electron gas subject to the Rashba SO coupling the intrinsic spin-Hall conductivity, σ_{sH}, is a universal constant ($\sigma_{\mathrm{sH}}=|e|/8\pi$,[3] where e is the electron charge) has been shown to be invalid even for an arbitrarily small concentration of impurities, which reduce σ_{sH} to zero.[4–8] At the same time, however, for other models of SO coupling such as, for example, the three-dimensional (3D) Dresselhaus model,[9] the Luttinger model for valence band holes,[10] or generalized Rashba models taking into account nonlinear momentum dependences of the SO interaction[11–13] or a non-quadratic unperturbed band spectrum,[14] σ_{sH} has been found to be robust against nonmagnetic impurity scatterings. This suggests that the vanishing of σ_{sH} is a peculiar feature of the linear Rashba model. This is also supported by rather general arguments that do not rely on the specific scattering process.[7,15]

Within the linear response theory, the vanishing of σ_{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.[4,5,7,8] 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 τ^{-1} associated with the current vertex (where τ is the electron lifetime due to impurities) is balanced by the factor τ arising from the product of two Green's 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. 4, 5, 7, and 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,[16] the surface states of metals and semimetals,[17,18] and even the heavy Fermion superconductor $\mathrm{CePt_3Si}$.[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.[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.[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 $E_F/E_0 \to \infty$, the spin-dependent part of the vertex function is generally not zero, and increases as E_F/E_0 decreases, eventually reaching unity as $E_F \to 0$. In this situation, the spin-Hall conductivity σ_{sH} would be nonzero if calculated along the lines of Refs. 4, 5, 7, and 8, in contradiction with the general arguments of Refs. 7 and 15. We resolve this inconsistency by showing that σ_{sH} is actually canceled by the contributions away from the Fermi surface, which have a magnitude equal to those on the Fermi surface, but opposite in sign.

We consider a 2D Rashba electron gas whose Hamiltonian is

$$H=\frac{\hbar^2k^2}{2m}+\gamma(k_x\sigma_y-k_y\sigma_x), \tag{1}$$

where m is the electron mass, $\mathbf{k}$ is the electron wave number, and γ is the SO coupling. The corresponding electron dispersion consists of two branches $E_k^s=\hbar^2(k+sk_0)^2/2m$ where s

$=\pm 1$ is the helicity number and $k_0=m\gamma/\hbar^2$. In the following, we parametrize the SO interaction by the Rashba energy $E_0=\hbar^2 k_0^2/2m$ that, for a clean system, corresponds to the minimum interband 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 $V(\mathbf{r})=V_{\text{imp}}\Sigma_i \delta(\mathbf{r}-\mathbf{R}_i)$, where the summation is performed over random positions $\mathbf{R}_i$ of the impurity scatterers with density n_i. The corresponding electron Green's function is a 2×2 matrix in the spin space,

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

where $G_s(k,i\omega_n)^{-1}=i\omega_n-E_k^s+\mu-\Sigma(i\omega_n)$ is the electron propagator in the helicity basis, μ 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,

$$\Sigma(i\omega_n)=\frac{1}{2\pi\tau N_0}\int\frac{d\mathbf{k}}{(2\pi)^2}G(\mathbf{k},i\omega_n)=\frac{1}{4\pi\tau N_0}\sum_{s=\pm}\int\frac{dk}{2\pi}kG_s(k,i\omega_n), \quad (3)$$

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

$$K_{sc}(i\omega_m)=T\sum_n\int\frac{d\mathbf{k}}{(2\pi)^2}\text{Tr}[j_s^y(\mathbf{k})G(\mathbf{k},i\omega_n+i\omega_m)\times J_c^x(\mathbf{k},i\omega_n+i\omega_m,i\omega_n)G(\mathbf{k},i\omega_n)]. \quad (5)$$

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

$$J_c^x(\mathbf{k},i\omega_l,i\omega_n)=j_c^x(\mathbf{k})+\frac{1}{2\pi\tau N_0}\int\frac{d\mathbf{k}'}{(2\pi)^2}G(\mathbf{k}',i\omega_l)\times J_c^x(\mathbf{k}',i\omega_l,i\omega_n)G(\mathbf{k}',i\omega_n), \quad (6)$$

where $j_c^x(\mathbf{k})=ev_x(\mathbf{k})=e\hbar k_x/m+e\gamma\sigma_y/\hbar$ is the bare charge current. Equation (6) can be rewritten as $J_c^x(\mathbf{k},i\omega_l,i\omega_n)=e\hbar k_x/m+e\gamma\Gamma(i\omega_l,i\omega_n)/\hbar$ where Γ represents the SO corrections to the charge current function. By using Eq. (2) and by taking advantage of the momentum independence of Σ, the correlation function K_{sc} reduces to

$$K_{sc}(i\omega_m)=i\frac{e\hbar^2\gamma}{4m}T\sum_n\Gamma_y(i\omega_n+i\omega_m,i\omega_n)\times B_1(i\omega_n+i\omega_m,i\omega_n)\equiv i\frac{e\hbar^2\gamma}{4m}T\sum_n\mathcal{K}(i\omega_n+i\omega_m,i\omega_n) \quad (7)$$

where Γ_y is the component of Γ proportional to σ_y, $\Gamma_y=\text{Tr}(\sigma_y\Gamma)/2$, which, by using Eq. (6), becomes

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

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

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

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

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

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,[22] leading to

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

where $f(x)=1/[\exp(x/T)+1]$ is the Fermi distribution function. When the spin-Hall conductivity is evaluated via Eq. (4), it is clear that the resulting σ_{sH} will be given by the sum of two contributions, σ_{sH}^{RA} and σ_{sH}^{RR}, 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, σ_{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 $f(\epsilon)$, therefore allowing for processes away from the Fermi surface. In Refs. 4, 5, 7, and 8 this term has been disregarded because in the large E_F limit it scales as $E_0/(\tau E_F^2)$,[4,7] and the spin-Hall conductivity has been approximated by the σ_{sH}^{RA} contribution alone, which at zero temperature reduces to

$$\sigma_{\mathrm{sH}}^{RA} = -\frac{e\hbar^2\gamma}{8\pi m}\Gamma_y^{RA}\int\frac{dk}{2\pi}k^2\sum_s sG_{-s}^R(k,0)G_s^A(k,0). \quad (13)$$

Here $G_s^{R(A)}$ is the retarded (advanced) Green's function and $\Gamma_y^{RA}=\Gamma_y(0+i\delta,0-i\delta)$ is the ladder vertex function (8) calculated at $i\omega_l=i\delta$ 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 (3) can be approximated as $\Sigma^R(\omega)=-i/2\tau$,[22] and the bubble term B_2 defined in Eq. (10) reduces to $B_2(i\delta,-i\delta)=-8\pi\tau N_0k_0$, which by using Eq. (8) leads to $\Gamma_y^{RA}=0$. This is the vertex cancellation mechanism pointed out in Refs. 4, 5, 7, and 8.

We reexamine now Eq. (13) by relaxing the hypothesis $E_F \gg E_0$. For practical purposes, we introduce an upper momentum cutoff k_c such that all the relevant momentum and energy scales are much smaller than the corresponding cutoff quantities, namely $k_0,k_F \ll k_c$, $E_F,E_0,1/\tau \ll E_c=\hbar^2k_c^2/2m$. After the analytical continuation, the integration over momenta in Eq. (3) can be performed analytically and the real axis self-energy is evaluated numerically by iteration. The obtained Σ is then substituted into Γ_y^{RA} and $\sigma_{\mathrm{sH}}^{RA}$, Eq. (13), whose momentum integration allows for an analytical evaluation due to the momentum independence of Σ. To explore the effect of varying E_F on the spin-Hall conductivity, we have first evaluated the Green's functions at a 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

$$n = \frac{1}{2E_c}\int_{-\infty}^{\infty}d\omega f(\omega)\sum_s\frac{N_s(\omega)}{N_0}, \quad (14)$$

where $N_s(\omega)=-(1/\pi)\int dk/2\pi k \,\mathrm{Im}\, G_s^R(k,\omega)$ 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 Γ_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 Γ_y^{RA} is negligibly small, confirming the results reported in Refs. 4, 5, 7, and 8. However, as $E_F\tau$ is decreased, Γ_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 $\sigma_{\mathrm{sH}}^{RA}$ is expected to be nonzero. This is indeed shown in Fig. 1(b) where $\sigma_{\mathrm{sH}}^{RA}$, Eq. (13), is plotted in units of $|e|/8\pi$ as a function of $E_F\tau$. The nonmonotonic behavior of $\sigma_{\mathrm{sH}}^{RA}$ is due to the competition between the increase of Γ_y^{RA} shown in Fig. 1(a) and the decrease of the integral appearing in Eq. (13) as $E_F\to 0$.

A nonvanishing spin-Hall conductivity in an impure 2D Rashba electron gas is at odds with the general arguments of Refs. 7 and 15, where σ_{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 $\sigma_{\mathrm{sH}}=\sigma_{\mathrm{sH}}^{RA}+\sigma_{\mathrm{sH}}^{RR}$, where

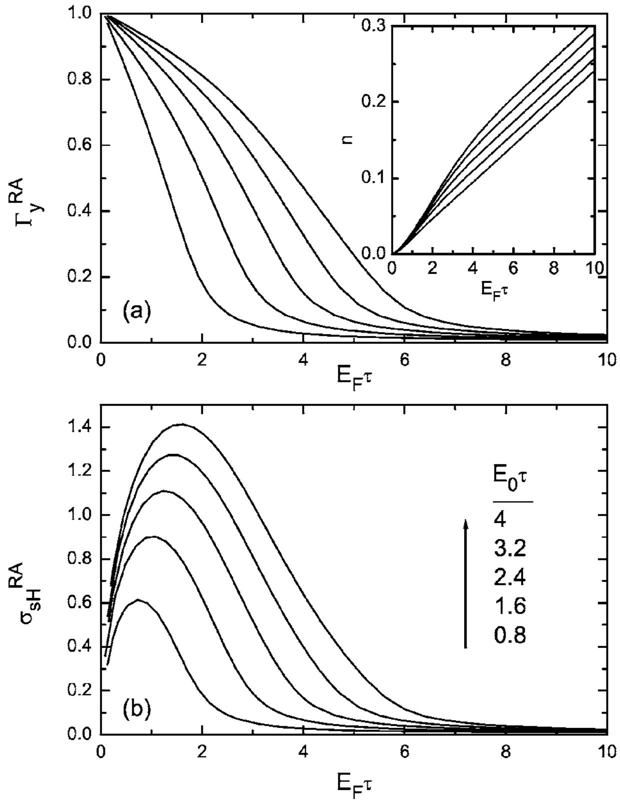

FIG. 1. (a) Spin-orbit vertex function Γ_y^{RA} as a function of $E_F\tau$ for different values of the spin-orbit energy E_0. The scattering time τ has been set equal to $\tau=80/E_c$, where E_c is the upper energy cutoff (see text). Inset: number electron density n of the interacting system as a function of $E_F\tau$. (b) The retarded-advanced part $\sigma_{\mathrm{sH}}^{RA}$ of the spin-Hall conductivity in units of $|e|/8\pi$ obtained from Eq. (13) for the same parameter values of (a).

$$\sigma_{\mathrm{sH}}^{RR} = \frac{e\hbar^2\gamma}{4\pi m}\mathrm{Im}\int_{-\infty}^{\infty}d\epsilon f(\epsilon)\Gamma_y^{RR}(\epsilon) \times \int\frac{dk}{2\pi}k^2\sum_s s\frac{dG_{-s}^R(k,\epsilon)}{d\epsilon}G_s^R(k,\epsilon), \quad (15)$$

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

Our numerical calculations of $\sigma_{\mathrm{sH}}^{RR}$, Eq. (15), are plotted in Fig. 2 (dashed lines) together with the corresponding $\sigma_{\mathrm{sH}}^{RA}$ results already plotted in Fig. 1(b). For all E_F/E_0 values, $\sigma_{\mathrm{sH}}^{RR}$ has the same magnitude of $\sigma_{\mathrm{sH}}^{RA}$ but with opposite sign, so that the resulting physical spin-Hall conductivity, $\sigma_{\mathrm{sH}}=\sigma_{\mathrm{sH}}^{RA}+\sigma_{\mathrm{sH}}^{RR}$ (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 (15) away from the Fermi surface, resolving therefore the concerns expressed in Ref. 11 about an only-on-Fermi-surface cancellation mechanism.

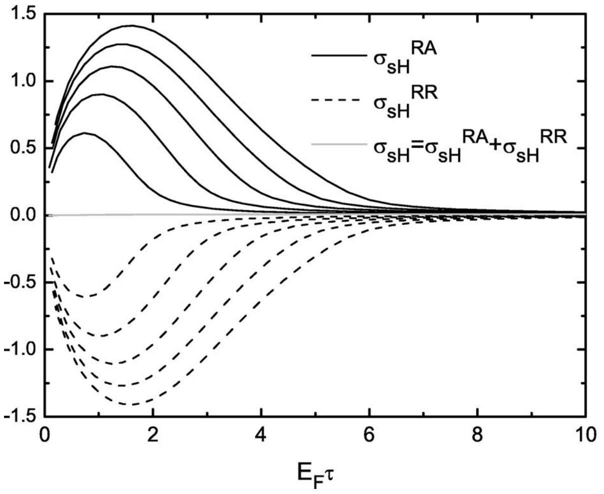

FIG. 2. The different cotributions to the spin-Hall conductivity for the same parameters of Fig. 1: $\sigma_{\mathrm{sH}}^{RA}$ (solid lines), $\sigma_{\mathrm{sH}}^{RR}$ (dashed lines), and the physical spin-Hall conductivity $\sigma_{\mathrm{sH}}=\sigma_{\mathrm{sH}}^{RA}+\sigma_{\mathrm{sH}}^{RR}$ (gray lines). All conductivities are given in units of $|e|/8\pi$.

However, on this point, a few remarks should be brought to attention. First, the cancellation between $\sigma_{\mathrm{sH}}^{RA}$ and $\sigma_{\mathrm{sH}}^{RR}$ suggests that, by suitable mathematical transformations, the (nominal) off-Fermi surface contribution (15) may be expressed as $-\sigma_{\mathrm{sH}}^{RA}$, 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 $\sigma_{\mathrm{sH}}^{RR}$ 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 $-\sigma_{\mathrm{sH}}^{RA}$. In this case, any variation from the linear Rashba model of (1) would result in $\sigma_{\mathrm{sH}}^{RA}$ and $\sigma_{\mathrm{sH}}^{RR}$ terms that 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. 7 and 15 about the vanishing of σ_{sH} apply only for model Hamiltonians of the type (1).

Before concluding, it is worth stressing that the results presented in this work could be relevant also for systems described by nonlinear Rashba or 3D Dresselhaus SO couplings, or by nonquadratic unperturbed electronic band structures. It is known that for such systems, the spin-Hall conductivity in the presence of momentum scattering is nonzero also for $E_F/E_0\to\infty$ because the SO vertex does not vanish.[9–14] Our results suggest, however, that even in this case, for finite E_F/E_0, a quantitatively reliable calculation of σ_{sH} should take into account also the off-Fermi surface contributions. This could be for example the case of the system studied in Ref. 18 where E_F is of the same order as E_0 and the unperturbed band spectrum is clearly nonquadratic.

In conclusion, we have calculated the spin-Hall conductivity σ_{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 $\sigma_{\mathrm{sH}}^{RA}$ to the spin-Hall conductivity. We have demonstrated that the physical spin-Hall conductivity σ_{sH} actually includes also contributions away from the Fermi surface, $\sigma_{\mathrm{sH}}^{RR}$, which are as large as those on the Fermi surface, but of opposite sign, leading to a vanishing σ_{sH} for arbitrary values of E_F/E_0. We expect that, given the arguments of Refs. 7 and 15, the mutual cancellation of $\sigma_{\mathrm{sH}}^{RA}$ and $\sigma_{\mathrm{sH}}^{RR}$ for $E_F<\infty$ holds true also beyond the self-consistent Born approximation employed here.

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