Thermally induced spin polarization in a magnetized two-dimensional electron gas with Rashba spin-orbit interaction

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(Received 13 November 2017; revised manuscript received 6 July 2018; published 10 August 2018)

The spin polarization induced by a temperature gradient (heat current) in a magnetized two-dimensional electron gas (2DEG) with a Rashba spin-orbit interaction is considered theoretically within the linear response theory. Using the Matsubara Green's function formalism, we calculate the temperature dependence of the spin polarization for arbitrary orientation of the exchange field. The limit of a nonmagnetic 2DEG (zero exchange field) is also considered. Role of vertex corrections is investigated, and physical mechanisms of the spin polarization emergence are discussed. For a magnetic system, we identify a term in the spin polarization that stems from the Berry curvature of the corresponding electronic bands.

DOI: 10.1103/PhysRevB.98.075307

I. INTRODUCTION

The spin-orbit interaction couples the orbital motion of an electron to its spin orientation. In conducting materials, this coupling leads to various transport phenomena like anomalous Hall and Nernst effects as well as their spin counterparts, i.e., spin Hall and spin Nernst effects. These phenomena enable pure electrical or pure thermal control of spin (magnetic) moments [1,2]. Indeed, the spin current induced by the spin Hall effect is widely functionalized as a spin torque (so called spin-Hall torque) exerted on a magnetic moment triggering a magnetic dynamics and/or magnetic switching when the spin current exceeds a certain critical value.

One of the other consequences of the spin-orbit interaction is the current-induced nonequilibrium spin polarization (CISP) of conduction electrons. This means effectively that the system can be magnetically polarized by an electric field, similarly as in the case of multiferroic (magnetoelectric) systems (albeit the former case involves a nonequilibrium magnetization). The phenomenon of CISP was predicted theoretically in the '70s [3,4] and later it was studied theoretically [5–13] and also experimentally [14–22] in various materials. The phenomenon of CISP can occur in nonmagnetic as well as in magnetic systems, provided they exhibit spin-orbit coupling. If the system is already magnetic in the equilibrium, the induced nonequilibrium spin polarization may couple to the local magnetization *via* the exchange interaction, leading to a spin torque exerted on the local magnetization [23–27].

Recently, it has been shown that not only external electric field but also a temperature gradient may lead to a spin-orbit driven spin polarization [12,28,29]. These results initiated an interesting discussion on the thermally induced spin-orbit torque and also on possibly new ways of magnetization switching as an alternative to switching by electrically induced spin transfer torque [30–32]. The physical mechanisms of the thermally induced spin polarization of conduction electrons

are different from that for electrically induced spin polarization, although there are some similarities. In the case of an electric field, the field drives electrons and their wave vectors experience a net change $\Delta \mathbf{k}$ along the driving force. The electron spins precess to fit the new orientations of the Rashba field creating different distributions of electrons with positive and negative wave-vector components along the electric field. Taking into account the spin precession and equilibrium spin orientations in the two electronic subbands, one finds a nonzero net component of the spin polarization along the in-plane axis normal to the electric field. In the case of a temperature gradient, there is no electrical (mechanical) force, but instead we have a statistical force. In the absence of a temperature gradient, the average spin is zero. For a finite temperature gradient, the local distributions of electrons with positive and negative wave-vector components are different. This is because colder electrons arrive at a given point from one side and hotter electrons from the other side. Due to different densities of states in the two Rashba subbands, a nonzero spin polarization along the axis y (in-plane and normal to the gradient) appears.

Although the spin-orbit torques induced by an electric current and a temperature gradient are attracting a great deal of attention experimentally, for a consistent theoretical description of the spin polarization some work is still needed. In this paper, we consider the heat-current-induced spin polarization of a magnetic two-dimensional electron gas (2DEG) with Rashba spin-orbit interaction. Such a model is fundamental for many devices based on magnetic semiconductor heterostructures. We also briefly reconsider the nonmagnetic limit. To find the spin polarization, we employ the Matsubara-Green's function formalism. Detailed numerical calculations show that the spin polarizability has a maximum in the range of chemical potentials where the modification of the electronic subbands, due to Rashba spin-orbit coupling, is large, i.e., in the vicinity of the band edge of the lower subband.

The paper is organized as follows. In Sec. II, we describe the model and formalism used to obtain some general formulas that allow us to calculate the spin polarization induced by a thermal gradient. In Sec. III, we present and discuss the results on the spin polarization in the absence of exchange field. Then, in Sec. IV, we include the exchange field and present detailed results for exchange field perpendicular to the plane of 2DEG as well as for its arbitrary orientation. In Sec. V, we comment on relations between electrically and thermally induced spin polarization and show that *y* components of spin polarizability may satisfy the Mott-like relation. Finally, in Sec. VI, we summarize our results and also present general conclusions.

II. MODEL AND METHOD

The 2DEG with spin-orbit interaction of the Rashba type and an arbitrarily oriented exchange field is captured by the Hamiltonian

$$H = \varepsilon_k \sigma_0 + H_{\rm R} + H_{\rm ex},\tag{1}$$

where $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ and $H_{\rm R}$ is the Rashba term,

$$H_{\rm R} = \alpha (k_y \sigma_x - k_x \sigma_y), \qquad (2)$$

with α being the Rashba parameter, while H_{ex} describes the exchange interaction

$$H_{\rm ex} = \mathbf{H} \cdot \boldsymbol{\sigma}, \tag{3}$$

where **H** is the effective exchange field (measured here in energy units). In the equations above, the matrices σ_0 and $\sigma = \{\sigma_x, \sigma_y, \sigma_z\}$ are the unit and Pauli matrices, respectively, defined in the spin space. In turn, k_x and k_y are the in-plane wave-vector components.

We consider the nonequilibrium spin polarization in the system driven by a statistical force, i.e., by the temperature gradient (heat current). We also assume the temperature gradient ∇T is small and uniform across the whole system, so that the average temperature T is basically constant on the scale of the carrier wavelengths. The study is also restricted to cases away from any thermal phase transitions in the considered temperature range. With these assumptions, we can employ a finite-temperature theory for the linear response of the system to a temperature gradient, meaning that the sample is already at some mean temperature and we seek its linear response when exposed to a small temperature gradient. Technically, we will resort to similar concepts such as those introduced by Luttinger [33] and Strinati et al. [34] by defining an auxiliary time-dependent vector field of frequency ω/\hbar , $\mathbf{A}(t) = \mathbf{A}(\omega) \exp(-i\omega t/\hbar)$, which is associated with the heat current density operator, $\hat{\mathbf{j}}^h = \frac{1}{2} [\hat{H} - \mu \sigma_0, \hat{\mathbf{v}}]_+$ (here μ denotes the chemical potential), so the perturbation term has the form

$$\hat{H}_{\mathbf{A}}^{\nabla T}(t) = -\hat{\mathbf{j}}^{h} \cdot \mathbf{A}(t).$$
(4)

The vector field is related to the temperature gradient *via* $\mathbf{A}(\omega) = \frac{\hbar}{i\omega}(-\frac{\nabla T}{T})$ [12,35–39]. For a temperature gradient along the axis *x* the perturbation $\hat{H}_{\mathbf{A}}^{\nabla T}(t)$ has the form $\hat{H}_{\mathbf{A}}^{\nabla T}(t) = -\hat{j}_{x}^{h} A_{x}(t)$.

Within the conditions stated above, the nonequilibrium spin polarization, viewed as a first-order response to the temperature gradient can be calculated within the Matsubara-Green's function formalism as

$$S_{\alpha}(i\omega_m) = \frac{1}{\beta} \sum_{\mathbf{k},n} \operatorname{Tr} \left\{ \hat{s}_{\alpha} G_{\mathbf{k}}(i\varepsilon_n + i\omega_m) \hat{H}_{\mathbf{A}}^{\nabla T}(i\omega_m) G_{\mathbf{k}}(i\varepsilon_n) \right\},$$
(5)

where $\beta = 1/k_B T$, \hat{s}_{α} is the α th component of the spin operator and $\hat{H}_{\mathbf{A}}^{\nabla T}(i\omega_m) = -\hat{j}_x^h A_x(i\omega_m)$ with the amplitude of the vector potential: $A_x(i\omega_m) = \frac{\hbar}{i(i\omega_m)}(-\frac{\nabla_x T}{T})$. Furthermore, $\varepsilon_n = (2n+1)\pi/\beta$ and $\omega_m = 2m\pi/\beta$ are the Matsubara energies, while $G_{\mathbf{k}}(i\varepsilon_n)$ are the Matsubara-Green's functions.

To sum over the Matsubara energies, we need to assume $k_BT > \Gamma = \hbar/2\tau$, where Γ is the imaginary part of the self-energy, while τ is the corresponding relaxation time. Then, upon performing the summation over the Matsubara energies [40,41], one finds the spin polarization induced by the temperature gradient in the following form:

$$S_{\alpha}(\omega) = \frac{\hbar}{\omega} \frac{\nabla_{x} T}{T} \operatorname{Tr} \sum_{\mathbf{k}} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \hat{s}_{\alpha} \\ \times \left(G_{\mathbf{k}}^{R}(\varepsilon + \omega) \hat{j}_{x}^{h} \Big[G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \Big] \\ + \Big[G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \Big] \hat{j}_{x}^{h} G_{\mathbf{k}}^{A}(\varepsilon - \omega) \Big).$$
(6)

The key steps of the derivation of the above formula are described elsewhere [38,42]. Equation (6) is our starting expression for further considerations.

Before calculating the spin polarization, we comment on the applicability range of the formalism used in this paper. At a finite T, the spin polarization is calculated as a linear response to $\nabla_x T/T$. Accordingly, we may write

$$S_{v}(\omega) = \chi_{v}(\omega)(\nabla_{x}T/T), \qquad (7)$$

where χ_y is the response function (in the following, it will be also referred to as the spin polarizability). In the present formalism, the response function can be calculated from the formula

$$\chi_{y}(\omega) = \frac{\hbar}{\omega} \operatorname{Tr} \sum_{\mathbf{k}} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \hat{s}_{\alpha} \Big(G_{\mathbf{k}}^{R}(\varepsilon + \omega) \hat{j}_{x}^{h} \\ \times \Big[G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \Big] \\ + \Big[G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \Big] \hat{j}_{x}^{h} G_{\mathbf{k}}^{A}(\varepsilon - \omega) \Big).$$
(8)

The limit $T \to 0$ needs a careful inspection. Our linear response approach requires that the statistical driving force $\nabla_x T/T$ is small. Moreover, the statistical force should disappear in the limit $T \to 0$. Thus, when $T \to 0$, $\nabla_x T/T$ should also tend to zero, $\nabla_x T/T \to 0$ for $T \to 0$. This results in zero spin polarization for the zero temperature limit, $S_y(T = 0) \to 0$ when $T \to 0$.

From the above discussion, it follows that the most convenient way to present the numerical results is simply to show the response function as $\chi_y = S_y/(\nabla_x T/T)$. Note, that even if the thermal spin polarizability χ_y is nonzero in the limit $T \rightarrow 0$, the corresponding spin polarization vanishes due to vanishing driving statistical force.

This can be also supported by the fact that the nonequilibrium spin polarization is not associated with the entropy generation, while the coefficients determining the polarization are not related to the kinetic coefficients. From an experimental point of view, it is of course more relevant to operate at finite temperatures and moderate temperature gradients that can be realized on the nanoscale. This is the range where our theory is useful.

In Appendix **B**, we present the explicit formulas for the kinetic coefficients, the entropy production, and the Onsager relations for the case of 2D systems with Rashba spin-orbit coupling in the magnetization field **M**. Analyzing these relations in connection with the obtained results, we come to the conclusion that the calculated thermally induced bulk polarization (i) does not contradict the Onsager relations, (ii) it does not lead to any unphysical divergences at $T \rightarrow 0$ (as explained above), and (iii) it is not related to the production of entropy. This makes it different from the known problem of orbital magnetization, where the surface currents should be accounted for to restore the Onsager relations, avoiding unphysical divergences at $T \rightarrow 0$ and obeying the third law of thermodynamics.

III. SPIN POLARIZATION IN A NONMAGNETIC 2DEG

Let us consider at first the case with zero exchange field, i.e., when the 2DEG is nonmagnetic. The Hamiltonian Eq. (1) reduces to the form

$$H = \varepsilon_k \sigma_0 + \alpha (k_y \sigma_x - k_x \sigma_y), \tag{9}$$

while the corresponding impurity-averaged retarded/advanced (R/A) Green's functions can be written as

$$G_{\mathbf{k}}^{R/A}(\varepsilon) = G_{\mathbf{k}0}^{R/A}(\varepsilon)\sigma_0 + G_{\mathbf{k}x}^{R/A}(\varepsilon)\sigma_x + G_{\mathbf{k}y}^{R/A}(\varepsilon)\sigma_y, \quad (10)$$

where

$$G_{\mathbf{k}0}^{R/A}(\varepsilon) = \frac{1}{2}[G_{+}(\varepsilon) + G_{-}(\varepsilon)], \qquad (11a)$$

$$G_{\mathbf{k}x}^{R/A}(\varepsilon) = \frac{\alpha k_y}{2\lambda_k} [G_+(\varepsilon) - G_-(\varepsilon)], \qquad (11b)$$

$$G_{\mathbf{k}y}^{R/A}(\varepsilon) = -\frac{\alpha k_x}{2\lambda_k} [G_+(\varepsilon) - G_-(\varepsilon)], \qquad (11c)$$

with $G_{\pm}^{R}(\varepsilon) = [\varepsilon + \mu - E_{\pm} + i\Gamma]^{-1}$, $G_{\pm}^{A}(\varepsilon) = [\varepsilon + \mu - E_{\pm} - i\Gamma]^{-1}$ and $E_{\pm} = \varepsilon_{k} \pm \lambda_{k}$ (with $\lambda_{k} = \alpha k$). Note, the relaxation rate (taken at the Fermi level) Γ in a nonmagnetic electron gas with Rashba interaction (assuming relaxation due to scattering on short-range impurities only) has the following explicit form: $\Gamma = n_{i}v_{0}^{2}\frac{m}{2\hbar^{2}} = \Gamma_{0}$ for $\mu > 0$ and $\Gamma = \Gamma_{0}\frac{n^{*}}{n}$ for $\mu < 0$. Here n^{*} and n stand for particle density for $\mu = 0$ and $\mu < 0$, respectively (for more details see, e.g., Ref. [38]). Treating Γ as a small fixed parameter, as done in this work, means that for each value of the chemical potential, the spin polarizability corresponds to a different impurity potential or different concentration of impurities. In the nonmagnetic case, this assumption is relevant for the negative chemical potentials; that is, for $0 < \mu < E_{\min}$ (where E_{\min} means the minimum of the lower energy branch).

A. Bare bubble approximation

The heat current operator corresponding to the Hamiltonian Eq. (9) has the explicit form

$$\hat{j}_{x}^{h} = \left((\varepsilon_{k} - \mu) \frac{\hbar k_{z}}{m} + \frac{\alpha^{2}}{\hbar} k_{x} \right) \sigma_{0} + \alpha \frac{\hbar}{m} k_{x} k_{y} \sigma_{x} - \left(\frac{\alpha}{\hbar} (\varepsilon_{k} - \mu) + \alpha \frac{\hbar}{m} k_{x}^{2} \right) \sigma_{y}.$$
(12)

Inserting Eqs. (10) to (12) into Eq. (6), we find that only the *y* component of the spin polarization is nonzero, namely

$$S_{y}^{T}(\omega) = \frac{\hbar}{\omega} \frac{\nabla_{x} T}{T} \int \frac{dk}{(2\pi)^{2}} \left(-\frac{\pi}{2} [2\varepsilon_{k}(\varepsilon_{k} - \mu) + \alpha^{2}k^{2}] S_{A} + \alpha \frac{\pi}{2} k [(\varepsilon_{k} - \mu) S_{B} + (3\varepsilon_{k} - \mu) S_{C}] \right), \quad (13)$$

where

$$S_{A} = I_{--}^{RA}(\omega) - I_{--}^{RR}(\omega) + I_{++}^{RR}(\omega) - I_{++}^{RA}(\omega) + I_{--}^{AA}(-\omega) - I_{++}^{AA}(-\omega) - I_{--}^{RA}(-\omega) + I_{++}^{RA}(-\omega),$$
(14)

$$S_{B} = I_{-+}^{RA}(\omega) - I_{-+}^{RR}(\omega) + I_{+-}^{RA}(\omega) - I_{+-}^{RR}(\omega) + I_{-+}^{AA}(-\omega) + I_{+-}^{AA}(-\omega) - I_{-+}^{RA}(-\omega) - I_{+-}^{RA}(-\omega),$$
(15)

$$S_{C} = I_{--}^{RA}(\omega) - I_{--}^{RR}(\omega) + I_{++}^{RA}(\omega) - I_{++}^{RR}(\omega) + I_{--}^{AA}(-\omega) + I_{++}^{AA}(-\omega) - I_{--}^{RA}(-\omega) - I_{++}^{RA}(-\omega).$$
(16)

Here we use the notation $I_{mn}^{XY}(\omega) = \int \frac{d\varepsilon}{2\pi} G_m^X(\varepsilon + \omega) G_n^Y(\varepsilon)$ and $I_{mn}^{XY}(-\omega) = \int \frac{d\varepsilon}{2\pi} G_m^X(\varepsilon) G_n^Y(\varepsilon - \omega)$ with $m, n = \{+, -\}$ and $X, Y = \{R, A\}$.

Upon integrating over ε and taking the limit $\omega \to 0$, we find the thermally induced spin polarization

$$S_{y} = -\frac{\hbar}{2\Gamma} \frac{\nabla_{x}T}{T} \int \frac{dk}{4\pi} \left(\varepsilon_{k}(\varepsilon_{k}-\mu) + \frac{1}{2}\alpha^{2}k^{2} \right)$$

$$\times [f'(E_{+}) - f'(E_{-})]$$

$$-\frac{\hbar}{2\Gamma} \frac{\nabla_{x}T}{T} \frac{\alpha}{2} \int \frac{dk}{4\pi} k(3\varepsilon_{k}-\mu)[f'(E_{+}) + f'(E_{-})]$$

$$-\alpha\hbar\Gamma \frac{\nabla_{x}T}{T} \int \frac{dk}{4\pi} k(\varepsilon_{k}-\mu) \frac{f'(E_{+}) + f'(E_{-})}{(E_{+}-E_{-})^{2} + (2\Gamma)^{2}}.$$
(17)

The first two terms in Eq. (17) are proportional to $\hbar/2\Gamma = \tau$, while the third term is proportional to Γ (or $1/\tau$). Thus, one may expect that the first two terms are dominant in general, while the third term is small. This, however, does not hold true in the low-temperature regime, where the first two terms cancel each other so that the dominant contribution (though very small) may stem from the third term, as shown below. The formula Eq. (17) is our general result for the spin polarization in the bare bubble approximation. Note, Γ is here a parameter which is constant (independent of energy/wave vector).

In the low-temperature regime, one can replace the derivatives of the Fermi distribution functions by appropriate Dirac delta-functions, and then the above expression can be integrated analytically. As already mentioned above, the first two terms in Eq. (17) then cancel each other, so the only contribution originates from the third term. Assuming $\mu > 0$ and taking into account the fact that the Dirac delta-functions for $\mu > 0$ can be expressed as

$$\delta(E_{\pm} - \mu) = \frac{m\,\delta(k - k_{\pm})}{\sqrt{2m\mu\hbar^2 + m^2\alpha^2}},\tag{18}$$

we find the thermal spin polarizability,

$$\chi_{y} = \frac{1}{2\Gamma} \frac{\alpha \hbar^{3}}{16\pi \sqrt{2m\mu \hbar^{2} + \alpha^{2}m^{2}}} \\ \times \left[\frac{k_{+}^{3} - \frac{2m\mu}{\hbar^{2}}k_{+}}{1 + (\alpha k_{+}/\Gamma)^{2}} + \frac{k_{-}^{3} - \frac{2m\mu}{\hbar^{2}}k_{-}}{1 + (\alpha k_{-}/\Gamma)^{2}} \right].$$
(19)

Note, that $\Gamma < k_B T$ in the above formula. Moreover, the formalism assumes well-defined quasiparticles, so $\Gamma \ll \alpha k_{\pm}$, where $k_{\pm} = \mp \frac{m\alpha}{\hbar^2} + \frac{1}{\hbar^2} \sqrt{m^2 \alpha^2 + 2m\mu \hbar^2}$ are the Fermi wave vectors in the two subbands. As a result, one finds

$$\chi_{y} = \frac{\hbar^{3}}{16\pi\sqrt{2m\mu\hbar^{2} + \alpha^{2}m^{2}}} \times \frac{\Gamma}{2} \left[k_{+} + k_{-} - \frac{2m\mu}{\hbar^{2}} \left(\frac{1}{k_{+}} + \frac{1}{k_{-}} \right) \right] = 0, \quad (20)$$

i.e., the spin polarizability vanishes in the low temperature regime.

When only one subband is occupied, $\mu < 0$, the Dirac Delta-functions for the E_{-} band read

$$\delta(E_{-}-\mu) = \frac{m[\delta(k-k_{-}^{+})+\delta(k-k_{-}^{-})]}{\sqrt{2m\mu\hbar^{2}+m^{2}\alpha^{2}}},$$
 (21)

where now $k_{-}^{\pm} = \frac{m\alpha}{\hbar^2} \pm \sqrt{2m\mu\hbar^2 + m^2\alpha^2}$. The spin polarizability is then given by the formula

$$\chi_{y} = \frac{1}{2\Gamma} \frac{\alpha \hbar^{3}}{16\pi \sqrt{2m\mu \hbar^{2} + \alpha^{2}m^{2}}} \\ \times \left[\frac{(k_{-}^{+})^{3} - \frac{2m\mu}{\hbar^{2}}k_{-}^{+}}{1 + (\alpha k_{-}^{+}/\Gamma)^{2}} + \frac{(k_{-}^{-})^{3} - \frac{2m\mu}{\hbar^{2}}k_{-}^{-}}{1 + (\alpha k_{-}^{-}/\Gamma)^{2}} \right], \quad (22)$$

and now may generally remain small but nonzero in the low-temperature regime for $\Gamma < k_B T$ and $\Gamma \ll \alpha k_-^{\pm}$.

B. Vertex correction

It is known that the impurity vertex corrections can have a significant impact on various physical quantities, like, for instance, on the spin Hall conductivity of a 2DEG with Rashba interaction. Therefore, we consider now the vertex corrections to the spin polarization.

The equation for the renormalized spin vertex reads

$$\bar{S}_{y} = \frac{\hbar}{2}\sigma_{y} + n_{i}v_{0}^{2}\int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}}G_{\mathbf{k}}^{A}(\varepsilon)\bar{S}_{y}G_{\mathbf{k}}^{R}(\varepsilon+\omega).$$
 (23)

We look for a solution of Eq. (23) in the following form: $\bar{S}_y = a\sigma_0 + b\sigma_x + c\sigma_y + d\sigma_z$. Then, from Eq. (23), we find that a = b = d = 0, while *c* is given by the following formula:

$$c = \frac{\hbar}{2} \left[1 - \frac{1}{2} \pi n_i V^2 \left(\mathcal{I}_{--}^{RA} + \mathcal{I}_{++}^{RA} + \mathcal{I}_{+-}^{RA} + \mathcal{I}_{-+}^{RA} \right) \right]^{-1}.$$
 (24)

Taking the above expression at the Fermi level ($\varepsilon = 0$) and assuming the limit of $\omega \rightarrow 0$, one finds

$$\bar{S}_{y} = \frac{\hbar}{2} \frac{1}{1 - \frac{1}{2}\pi n_{i} v_{0}^{2} (\mathcal{I}_{1} + \mathcal{I}_{2})} \sigma_{y}, \qquad (25)$$

where the integrals $\mathcal{I}_{1,2}$ are defined as

$$\begin{aligned} \mathcal{I}_{1} &= \int \frac{dkk}{(2\pi)^{2}} \bigg[\frac{1}{(\mu - E_{+})^{2} + \Gamma^{2}} + \frac{1}{(\mu - E_{-})^{2} + \Gamma^{2}} \bigg], \ (26) \\ \mathcal{I}_{2} &= \Re \int \frac{dkk}{(2\pi)^{2}} \frac{E_{-} - E_{+} - 2i\Gamma}{(E_{-} - E_{+})^{2} + (2\Gamma)^{2}} \\ &\times \bigg[\frac{\mu - E_{-} + i\Gamma}{(\mu - E_{-})^{2} + \Gamma^{2}} - \frac{\mu - E_{+} - i\Gamma}{(\mu - E_{+})^{2} + \Gamma^{2}} \bigg] \\ &+ \int \frac{dkk}{(2\pi)^{2}} \frac{E_{+} - E_{-} - 2i\Gamma}{(E_{+} - E_{-})^{2} + (2\Gamma)^{2}} \\ &\times \bigg[\frac{\mu - E_{+} + i\Gamma}{(\mu - E_{+})^{2} + \Gamma^{2}} - \frac{\mu - E_{-} - i\Gamma}{(\mu - E_{-})^{2} + \Gamma^{2}} \bigg]. \ (27) \end{aligned}$$

It is convenient to introduce the parameter β by the following equality:

$$\frac{1}{2}\pi n_i v_0^2 (\mathcal{I}_1 + \mathcal{I}_2) \equiv \frac{1}{2} + \beta.$$
(28)

This parameter can be determined from Eqs. (26) and (27). Accordingly, we may write the renormalized vertex function in the following form:

$$\bar{S}_y = \hat{s}_y \frac{2}{1 - 2\beta},\tag{29}$$

or, alternatively,

$$\bar{S}_y = \hat{s}_y + \delta \hat{s}_y \equiv \hat{s}_y + \gamma \frac{\hbar}{2} \sigma_y, \qquad (30)$$

where $\gamma = \frac{1+2\beta}{1-2\beta}$. Thus, the spin polarization with the vertex correction included can be written as

$$S_{y}^{\text{tot}} = S_{y} + \Delta S_{y}, \qquad (31)$$

where S_{ν} is given by Eq. (17) while ΔS_{ν} is given by the formula

$$\Delta S_{y} = -\frac{\hbar}{\omega} \frac{\nabla_{x} T}{T} \operatorname{Tr} \int \frac{d^{2} \mathbf{k}}{(2\pi)^{2}} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \delta \hat{s}_{y} \\ \times \left(G_{\mathbf{k}}^{R}(\varepsilon + \omega) \hat{j}_{x}^{h} G_{\mathbf{k}}^{A}(\varepsilon) - G_{\mathbf{k}}^{R}(\varepsilon) \hat{j}_{x}^{h} G_{\mathbf{k}}^{A}(\varepsilon - \omega) \right). (32)$$

Upon integration over ε in Eq. (32), the final formula for the total spin polarization (including vertex correction) reads

$$S_{y} = -\frac{\hbar}{2\Gamma} \frac{\nabla_{x} T}{T} (1+\gamma) \\ \times \left\{ \int \frac{dk}{4\pi} \left(\varepsilon_{k} (\varepsilon_{k} - \mu) + \frac{1}{2} \alpha^{2} k^{2} \right) [f'(E_{+}) - f'(E_{-})] \right. \\ \left. + \frac{\alpha}{2} \int \frac{dk}{4\pi} k (3\varepsilon_{k} - \mu) [f'(E_{+}) + f'(E_{-})] \right. \\ \left. + 2\alpha\Gamma^{2} \int \frac{dk}{4\pi} k (\varepsilon_{k} - \mu) \frac{f'(E_{+}) + f'(E_{-})}{(E_{+} - E_{-})^{2} + (2\Gamma)^{2}} \right\}.$$
(33)

The vertex renormalization leads in effect to a multiplication of the spin polarization obtained in the bare bubble approximation [given by Eq. (17)] by a factor $1 + \gamma = 2/(1 - 2\beta)$, which can be found from Eqs. (26) to (28). This renormalization factor is equal to that found in the case of the spin polarization induced by an external electric field [42].

Some analytical results for β (and thus also for γ) can be derived for small Γ , when the integrals Eqs. (26) and (27) take on the form

$$\mathcal{I}_1 \cong \frac{1}{2\Gamma} \int \frac{dkk}{2\pi} [\delta(E_+ - \mu) + \delta(E_- - \mu)], \qquad (34)$$

$$\mathcal{I}_{2} \cong \int \frac{dkk}{2\pi} \frac{2\Gamma}{(2\alpha k)^{2} + (2\Gamma)^{2}} [\delta(E_{+} - \mu) + \delta(E_{-} - \mu)].$$
(35)

The parameter β is then given by the formula

$$\beta = \frac{\hbar^2}{4\sqrt{2m\mu\hbar^2 + m^2\alpha^2}} \left[\frac{k_+}{1 + \left(\frac{\alpha k_+}{\Gamma}\right)^2} + \frac{k_-}{1 + \left(\frac{\alpha k_-}{\Gamma}\right)^2} \right]$$
(36)

for $\mu > 0$, and

$$\beta = \frac{\hbar^2}{4\sqrt{2m\mu\hbar^2 + m^2\alpha^2}} \left[\frac{k_-^+}{1 + \left(\frac{\alpha k_-^-}{\Gamma}\right)^2} + \frac{k_-^-}{1 + \left(\frac{\alpha k_-^-}{\Gamma}\right)^2} \right] (37)$$

for $\mu < 0$. Having found β , we have also the parameter γ .

C. Numerical results

The numerical results presented here are for the low impurity case where the parameter Γ is very small. The parameter γ is then roughly equal to 1, so the results including the vertex correction can be obtained from those derived in the single loop approximation upon multiplying the latter by a factor roughly equal to 2.

In Fig. 1, we show the total (with vertex corrections included) thermal response function due to a temperature gradient in a nonmagnetic system. The only nonzero component of spin polarization in the absence of the exchange field is the in-plane component perpendicular to $\nabla_x T$, i.e., the component $S_{\rm v}$. Figures 1(a) and 1(b) show the spin polarizability as a function of chemical potential for different Rashba coupling constants and temperatures, respectively. Note, the parameter Γ assumed in Fig. 1 is 0.005 meV, thus the minimal temperature for which our formalism works properly is approximately 0.06 K. When T increases, the spin polarization also increases and has a maximum for the Fermi level around the bottom of the lower electronic band. The spin polarizability as a function of the chemical potential has then the form of a narrow and asymmetric peak. When T increases further, the maximum value of the spin polarization saturates, while the peaks become broader. The spin polarizability is plotted also as a function of temperature from $T_{\rm min} = 0.06$ K up to 250 K for fixed chemical potential, μ , [Fig. 1(c)] and a fixed Rashba parameter, α [Fig. 1(d)]. Evidentl, y χ_v is diminished when the temperature tends to zero, and for higher values of T it behaves as a linear function of T. This is consistent with the physical mechanism of the thermally induced spin polarization. Three ingredients of this mechanism are important: (i) the spin orientation in



FIG. 1. The y component of the thermally induced spin polarizability in a nonmagnetic electron gas shown as a function of the chemical potential for the indicated Rashba coupling constant and temperatures (a), (b); as a function of temperature for the indicated chemical potentials and the Rashba parameters (c), (d). Other parameters as indicated, whereas $m = 0.07m_0$, and $\Gamma = 5 \cdot 10^{-3}$ meV.

the two electronic subbands is determined by the Rashba coupling and the total spin in the equalibrium vanishes in each subband. (ii) Rashba splitting of the electronic bands introduces some asymmetry in the density of states of the two subbands, and (iii), due to the temperature gradient, there is an imbalance in the spin flowing into a certain region from the colder and hotter sides. All this leads to a net spin polarization. Moreover, this also explains why the maximum of the spin polarization appears close to the bottom of the lower band. The latter takes place because the modifications in the electronic structure by the Rashba coupling are most significant there. In turn, the broadening of the peaks with increasing temperature is a consequence of the broadening of the Fermi distribution function. The almost symmetrical shape is due to the assumption of a constant chemical potential. In other words, our system is assumed to be attached to two (left and right) electronic reservoirs where the electrons are described by the chemical potential μ . Thus, even if the chemical potential is below the band edge in 2DEG, the electrons can be injected into the system from the reservoirs when the temperature is sufficiently high.

Increasing the Rashba parameter, the spin polarization also increases. Moreover, the band edge of the lower band is shifted down so that the peak in the spin polarization slightly shifts towards lower values of the chemical potential. This behavior is shown in Fig. 1(a), where different curves correspond to different values of the parameter α . The interplay of this shift and of the increase of the maximum spin polarization with α leads to some nonmonotonous behavior of the spin polarization with the Rashba parameter, especially at higher values of μ , where the spin polarization is already very small.

IV. SPIN POLARIZATION IN THE PRESENCE OF EXCHANGE FIELD

Considering the full Hamiltonian Eq. (1) with the exchange term H_{ex} , we cast the exchange field in spherical coordinates $\mathbf{H} = (H_x, H_y, H_z)$ as

$$H_x = JM\sin\theta\cos\xi,\tag{38a}$$

$$H_{y} = JM\sin\theta\sin\xi, \qquad (38b)$$

$$H_z = JM\cos\theta, \qquad (38c)$$

where J is a parameter proportional to the exchange constant and M is the effective magnetization which in general depends on the temperature according to Bloch's law, $M(T) = M_0[1 - (T/T_c)^{3/2}]$ (with T_c being the Curie temperature and M_0 stands for the magnetization at T = 0). The angles θ and ξ are the polar and the azimuthal angles in spherical coordinates.

The eigenvalues of the Hamiltonian Eq. (1) are

$$E_{\pm} = \varepsilon_k \pm \lambda_k, \tag{39}$$

where now the parameter $\lambda_{\mathbf{k}}$ is defined as $\lambda_{\mathbf{k}} = \sqrt{J^2 M^2 + \alpha^2 k^2 + 2JM\alpha} \sin \theta (k_x \sin \xi - k_y \cos \xi)$. The retarded/advanced Green's functions corresponding to the Hamiltonian Eq. (1) read

$$G_{\mathbf{k}}^{R/A}(\varepsilon) = G_{\mathbf{k}0}^{R/A}(\varepsilon)\sigma_0 + G_{\mathbf{k}x}^{R/A}(\varepsilon)\sigma_x + G_{\mathbf{k}y}^{R/A}(\varepsilon)\sigma_y + G_{\mathbf{k}z}^{R/A}(\varepsilon)\sigma_z, \qquad (40)$$

where

$$G_{\mathbf{k}0}^{R/A}(\varepsilon) = \frac{1}{2} [G_{+}(\varepsilon) + G_{-}(\varepsilon)], \qquad (41a)$$
$$G_{\mathbf{k}x}^{R/A}(\varepsilon) = \frac{1}{2\lambda_{\mathbf{k}}} (\alpha k_{y} + H \sin\theta\cos\xi) [G_{+}(\varepsilon) - G_{-}(\varepsilon)], \qquad (41b)$$

$$G_{\mathbf{k}y}^{R/A}(\varepsilon) = -\frac{1}{2\lambda_{\mathbf{k}}}(\alpha k_x - H\sin\theta\sin\xi)[G_{+}(\varepsilon) - G_{-}(\varepsilon)],$$
(41c)

$$G_{\mathbf{k}z}^{R/A}(\varepsilon) = \frac{1}{2\lambda_{\mathbf{k}}} H \cos\theta [G_{+}(\varepsilon) - G_{-}(\varepsilon)], \qquad (41d)$$

while $G_{\pm}^{R}(\varepsilon) = [\varepsilon + \mu - E_{\pm} + i\Gamma]^{-1}$ and $G_{\pm}^{A}(\varepsilon) = [\varepsilon + \mu - E_{\pm} - i\Gamma]^{-1}$. Note, we assumed Γ is a constant parameter for both subbands. Apart from this, the expansion of the Green function in Pauli materices includes now the term proportional to σ_{z} , which was absent in the case of no exchange field, see Eq. (8).

The operator of the heat current density is

$$\hat{j}_{x}^{h} = j_{x0}^{h} \sigma_{0} + j_{xx}^{h} \sigma_{x} + j_{xy}^{h} \sigma_{y} + j_{xz}^{h} \sigma_{z}, \qquad (42)$$

where

$$j_{x0}^{h} = \left((\varepsilon_{k} - \mu) \frac{\hbar k_{x}}{m} + \frac{\alpha}{\hbar} (\alpha k_{x} - H_{y}) \right), \quad (43a)$$

$$j_{xx}^{h} = \frac{\hbar}{m} k_x (\alpha k_y + H_x).$$
(43b)

$$j_{xy}^{h} = \left(\frac{\alpha}{\hbar}(\varepsilon_{k} - \mu) + \frac{h}{m}k_{x}(\alpha k_{x} - H_{y})\right), \quad (43c)$$

$$j_{xz}^{h} = -\frac{h}{m}k_{x}H_{z}\sigma_{z}.$$
(43d)

A. General formula for the components of the spin polarization

In this section, we present some general formulas for the spin polarization. Inserting Eqs. (40)–(42) into Eq. (6) and taking the trace and integrating over ε we obtain the following general formulas for the spin polarization:

$$S_{x} = \hbar \frac{\nabla_{x}T}{T} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \left\{ \frac{1}{2\Gamma} \left[\frac{\hbar^{2}k_{x}}{2m\lambda_{\mathbf{k}}} (\varepsilon_{k} - \mu) + \frac{\alpha}{2\lambda_{\mathbf{k}}} (\alpha k_{x} - H_{y}) \right] (\alpha k_{y} + H_{x}) [f'(E_{+}) - f'(E_{-})] \right. \\ \left. + \alpha(\varepsilon_{k} - \mu) \left[\frac{1}{\Gamma} (\alpha k_{x} - H_{y}) (\alpha k_{y} + H_{x}) - \frac{\Gamma^{2}}{\lambda^{2}} H_{z} \right] \frac{f'(E_{+}) + f'(E_{-})}{(2\lambda_{\mathbf{k}})^{2} + (2\Gamma)^{2}} \right. \\ \left. + \frac{1}{2\Gamma} \frac{\hbar^{2}k_{x}}{2m} (\alpha k_{y} + H_{x}) [f'(E_{+}) + f'(E_{-})] + \alpha H_{z} \frac{\varepsilon_{k} - \mu}{4\lambda_{\mathbf{k}}^{3}} [f(E_{+}) - f(E_{-})] \right\},$$

$$S_{y} = \hbar \frac{\nabla_{x}T}{T} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \left\{ -\frac{1}{2\Gamma} \left[\frac{\hbar^{2}k_{x}}{2m\lambda_{\mathbf{k}}} (\varepsilon_{k} - \mu) + \frac{\alpha}{2\lambda_{\mathbf{k}}} (\alpha k_{x} - H_{y}) \right] (\alpha k_{x} - H_{y}) [f'(E_{+}) - f'(E_{-})] \right\}$$

$$\left. - \frac{1}{2\Gamma} \left[\frac{\alpha}{2\lambda_{\mathbf{k}}^{2}} (\varepsilon_{k} - \mu) (\alpha k_{x} - H_{y}) + \frac{\hbar^{2}k_{x}}{2m} \right] (\alpha k_{x} - H_{y}) [f'(E_{+}) + f'(E_{-})] \right]$$

$$+\frac{\alpha}{2}(\varepsilon_{k}-\mu)\left[\frac{(\alpha k_{x}-H_{y})^{2}}{\lambda_{k}^{2}}-1\right]\frac{2\Gamma}{(2\lambda_{k})^{2}+(2\Gamma)^{2}}[f'(E_{+})+f'(E_{-})]\bigg\},$$
(45)

$$S_{z} = \hbar \frac{\nabla_{x} T}{T} \int \frac{d^{2} \mathbf{k}}{(2\pi)^{2}} \Biggl\{ \frac{1}{2\Gamma} \Biggl[\frac{\hbar^{2} k_{x}}{2m\lambda_{\mathbf{k}}} (\varepsilon_{k} - \mu) + \frac{\alpha}{2\lambda_{\mathbf{k}}} (\alpha k_{x} - H_{y}) \Biggr] H_{z}[f'(E_{+}) - f'(E_{-})] + \alpha (\varepsilon_{k} - \mu) \Biggl[\frac{\Gamma^{2}}{\lambda^{2}} (\alpha k_{y} + H_{x}) + \frac{1}{\Gamma} H_{z} (\alpha k_{x} - H_{y}) \Biggr] \frac{f'(E_{+}) + f'(E_{-})}{(2\lambda_{\mathbf{k}})^{2} + (2\Gamma)^{2}} + \frac{1}{2\Gamma} \frac{\hbar^{2} k_{x}}{2m} H_{z}[f'(E_{+}) + f'(E_{-})] - \alpha (\alpha k_{y} + H_{x}) \frac{\varepsilon_{k} - \mu}{4\lambda_{\mathbf{k}}^{3}} [f(E_{+}) - f(E_{-})] \Biggr\}.$$
(46)



FIG. 2. The *x* and *y* components of the spin polarizability in a magnetic 2DEG. The upper panel (a), (c), (e), (g) corresponds to the χ_x component while the lower one (b), (d), (f), (h) to the χ_y component. The dependence on the chemical potential (a)–(d), the magnitude of the exchange field *JM* (e), (f) and the temperature *T* (g), (h) are shown for indicated parameters, and for $\Gamma = 5 \cdot 10^{-3}$ meV, $m = 0.07m_0$.

In the following, these formulas will be used to calculate numerically the spin polarization for a general orientation of the exchange field. The formulas simplify under some specific situations. Especially interesting is when the exchange field is normal to the plane of 2DEG, so we will analyze in detail this particular situation.

B. Exchange field perpendicular to the plane of 2DEG

1. Single loop approximation

When the exchange field is oriented perpendicularly to the surface of the two-dimensional gas we obtain

$$S_{x} = \alpha \hbar \frac{\nabla_{x} T}{T} H_{z} \int \frac{d^{2} \mathbf{k}}{(2\pi)^{2}} \left\{ -(\varepsilon_{k} - \mu) \frac{\Gamma^{2}}{\zeta^{2}} \frac{f'(E_{+}) + f'(E_{-})}{(2\zeta)^{2} + (2\Gamma)^{2}} + \frac{\varepsilon_{k} - \mu}{(2\zeta)^{2}} [f(E_{+}) - f(E_{-})] \right\},$$
(47)

$$S_{y} = \hbar \frac{\nabla_{x} T}{T} \frac{1}{2\Gamma} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} \left\{ -\frac{\hbar}{2\zeta} \left[\alpha \frac{\hbar k_{x}^{2}}{m} (\varepsilon_{k} - \mu) + \frac{\alpha}{\hbar} \alpha^{2} k_{x}^{2} \right] \right.$$

$$\times \left[f'(E_{+}) - f'(E_{-}) \right] - \frac{\hbar}{2\zeta^{2}} \left[\frac{\alpha}{\hbar} (\varepsilon_{k} - \mu) \alpha^{2} k_{x}^{2} + \alpha \frac{\hbar k_{x}^{2}}{m} \zeta^{2} \right]$$

$$\times \left[f'(E_{+}) + f'(E_{-}) \right] + \frac{\alpha}{2} (\varepsilon_{k} - \mu) \left[\frac{\alpha^{2} k_{x}^{2}}{\zeta^{2}} - 1 \right]$$

$$\times \frac{f'(E_{+}) + f'(E_{-})}{1 + (\zeta/\Gamma)^{2}} \right\}, \qquad (48)$$

$$S_z = 0, (49)$$

where ζ is defined as $\sqrt{J^2 M^2 + \alpha^2 k^2}$. Now, the component normal to the plane of 2DEG (i.e., along the exchange field) vanishes exactly. The in-plane component normal to the temperature gradient is modified by the exchange field, and

additionally the component along the temperature gradient (S_x) appears.

For clean systems, the S_x component is described only by the second line of Eq. (47) which does not depend on relaxation processes. Indeed, for $\Gamma \rightarrow 0$, only topological term survives and S_x may be rewritten in the following form:

$$S_x = -\frac{\hbar}{2} \frac{\nabla_x T}{T} \sum_n \int \frac{d^2 \mathbf{k}}{(2\pi)^2} f(E_n) \frac{\varepsilon_k - \mu}{\alpha} \mathcal{B}_z^n(\mathbf{k}), \quad (50)$$

where $\mathcal{B}_{z}^{n}(\mathbf{k}) = \mp \frac{\alpha^{2} H_{z}}{2\zeta^{2}}$ is the Berry curvature for the *n*th subband (n = + and n = -). In the low-temperature limit, the integrals in the above equations can be calculated analytically, so the spin polarizability for small relaxation rate can be expressed as follows:

$$\chi_{x} = \frac{\hbar^{3} H_{z}}{16\pi m\alpha^{3}} \bigg[\zeta_{+} - \zeta_{-} + \bigg(H_{z}^{2} + 2m\alpha^{2} \frac{\mu}{\hbar^{2}} \bigg) \frac{\zeta_{-} - \zeta_{+}}{\zeta_{+} \zeta_{-}} \bigg],$$
(51)

$$\chi_{y} = \frac{\hbar}{8\pi} \frac{\alpha}{\Gamma} \bigg\{ \frac{\nu_{+}}{2\zeta_{+}} [2\varepsilon_{k+}(\varepsilon_{k+} - \mu) + \alpha^{2}k_{+}^{2}] \\ - \frac{\nu_{-}}{2\zeta_{-}} [2\varepsilon_{k-}(\varepsilon_{k-} - \mu) + \alpha^{2}k_{-}^{2}] + [\nu_{+}\varepsilon_{k+} + \nu_{-}\varepsilon_{k-}] \bigg\},$$
(52)

where $\zeta_{\pm} = \zeta(k_{\pm})$, $\varepsilon_{k_{\pm}} = \varepsilon_k(k = k_{\pm})$ and the density of states $\nu_{\pm} = \nu(k = k_{\pm})$ with k_{\pm} standing for the Fermi wave vector corresponding to the E_{\pm} branch, respectively, $k_{\pm} = \frac{\sqrt{2m}}{\hbar^2} \sqrt{m\alpha^2 + \mu\hbar^2} \mp \sqrt{m^2\alpha^4 + 2m\alpha^2\hbar^2\mu + H_z^2\hbar^4}$. The results above, although analytical, are not very transparent because the Fermi wave vectors have rather entangled form.



FIG. 3. The impurity vertex correction plotted as a function of the Rashba coupling constant α and the exchange field H_z (a), and as a function of the chemical potential μ and the exchange field (b). The cross sections of these density plots are presented in (c) and (d), respectively.

Thus, we discuss below numerical results obtained based on Eqs. (47) and (48) for arbitrary temperatures and small Γ .

The corresponding results are shown in Fig. 2. The component S_y , which is the only nonvanishing component in the nonmagnetic case, is modified by the exchange field (see the lower panel in Fig. 2). This modification is significant especially for chemical potentials inside the energy gap. Such behavior is in agreement with other theoretical results obtained recently for oxide perovskites [43]. Additionally, the S_x component appears (see the upper panel in Fig. 2).

Consider first the component S_y . Due to the modified electronic spectrum by the exchange field, the spin polarization depends remarkably on JM. The magnitude of the negative peak of S_v decreases with increasing JM_0 . Furthermore, the width of the peaks increases with increasing JM_0 ; besides, due to a gap of magnitude 2JM created by the exchange field at k = 0, the spin polarization changes sign and is positive in a certain range of positive chemical potentials, see Fig. 2(b) (right of the main negative peak). These features are also clearly seen in Figs. 2(f) and 2(g). The temperature dependence is qualitatively similar to that in the nonmagnetic case, see Fig. 3(d). In turn, the component S_x is solely due to the exchange field and is roughly one order of magnitude smaller than the S_v component (cf. upper and lower panels in Fig. 2). The dependence of the spin polarization on the chemical potential, the exchange field, and the Rashba parameter is qualitatively similar to that of the S_{y} component, so we will not describe it in more detail.

The physical mechanism of the y component of the spin polarization is similar to that in the nonmagnetic case. The

appearance of the *x* component, in turn, is associated with the modification of the electronic band structure by the exchange field, and especially the modification of the corresponding spin structure. The modified electronic bands exhibit a Berry curvature which is related to a Berry phase. This in turn may be represented by a magnetic field normal to the plane of 2DEG. When the temperature gradient is along the *x* axis, then this magnetic field enforces a nonzero *x* component of the total spin of electrons with a positive (negative) k_x . However, the temperatures of the electrons entering a given point from x > 0 (x < 0) are different and therefore the average *x* components of the spin entering a given point from x > 0 (x < 0) are different, which gives rise to a nonzero *x* component of the spin density.

2. Impurity vertex correction

Now, we consider the influence of the impurity vertex correction on the thermally induced spin polarization. The self-consistent equation for the renormalized spin vertex function (x and y components) reads

$$\Xi_{i} = \sigma_{i} + n_{i} v_{0}^{2} \int \frac{d^{2}\mathbf{k}}{(2\pi)^{2}} G_{\mathbf{k}}^{A}(\varepsilon) \Xi_{i} G_{\mathbf{k}}^{R}(\varepsilon), \qquad (53)$$

for i = x, y. Assuming solution in the form

$$\Xi_i = a_i \sigma_0 + b_i \sigma_x + c_i \sigma_y + d_i \sigma_z, \tag{54}$$

we find the following set of algebraic equations for the coefficients $a_i - d_i$:

$$a_i = d_i F_0^{(1)} + a_i F_0^{(2)}, (55)$$

$$b_i = 1\delta_{ix} + c_i F_x^{(1)} + b_i F_x^{(2)}, (56)$$

$$c_i = 1\delta_{iy} + b_i F_y^{(1)} + c_i F_y^{(2)},$$
(57)

$$d_i = a_i F_z^{(1)} + d_i F_z^{(2)}, (58)$$

where

$$F_x^{(1)} = -iH_z n_i v_0^2 \int \frac{dkk}{4\pi} \frac{1}{\zeta} [G_-^R G_-^A - G_+^R G_+^A], \quad (59)$$

$$F_x^{(2)} = F_x^{(2a)} + F_x^{(2b)} + F_x^{(2c)},$$
(60)

$$F_x^{(2a)} = n_i v_0^2 \int \frac{dkk}{4\pi} [G_-^R G_+^A + G_+^R G_-^A], \qquad (61)$$

$$F_x^{(2b)} = n_i v_0^2 \int \frac{dkk}{4\pi} \frac{\alpha^2 k^2}{2\zeta^2} [G_-^R G_-^A + G_+^R G_+^A], \quad (62)$$

$$F_x^{(2c)} = -n_i v_0^2 \int \frac{dkk}{4\pi} \frac{\alpha^2 k^2}{2\zeta^2} [G_-^R G_+^A + G_+^R G_-^A], \quad (63)$$

and $F_0^{(1)} = F_z^{(1)}$, $F_y^{(1)} = -F_x^{(1)}$, $F_y^{(2)} = F_x^{(2)}$. From the solution of the above set of equations, we find

From the solution of the above set of equations, we find that the vertex renormalization leads to a multiplication of the x and y spin operators by the parameter

$$b_x = c_y = \kappa = \frac{1 - F_x^{(2)}}{\left(1 - F_x^{(2)}\right)^2 + \left(F_x^{(1)}\right)^2},\tag{64}$$

Thus, $\hat{s}_x = \frac{\hbar}{2}\sigma_x \rightarrow S_x = \kappa \hat{s}_x$ and $\hat{s}_y = \frac{\hbar}{2}\sigma_y \rightarrow S_y = \kappa \hat{s}_y$. In other words, the numerical and analytical results obtained



FIG. 4. The three components of the thermally induced spin polarization as a function of the polar and azimuthal angles describing the orientation of the exchange field. The right panel presents some cross-sections of the density plots shown in the left panel. The other parameters are as follows: $m = 0.07m_0$, $\alpha = 2 \cdot 10^{-11}$ eVm, and $\Gamma = 5 \cdot 10^{-3}$ meV.

in the single loop approximation should be multiplied by a constant factor given by Eq. (64). This factor varies between 1 and 2, depending on which interaction dominates: Rashba or exchange one. The interplay between the spin-orbit coupling and the exchange interaction is clearly seen in Fig. 3, where the coefficient κ is plotted as a function of the Rashba constant α and the exchange field H_z for a fixed chemical potential, $\mu = 5 \text{ meV}$ [Figs. 3(a) and 3(c)]. We also show the dependence of κ on the chemical potential and the exchange field for $\alpha = 20 \text{ meV}\mu\text{m}$, Figs. 3(b) and 3(d). When the exchange field is zero, the coefficient κ is equal to 2 and decreases with increasing H_{z} . Additionally, there is a sharp jump (note that this is not a discontinuity) for the chemical potential corresponding to the bottom of the upper subband. When only a single subband is occupied, κ is almost independent of the exchange field.

C. Exchange field arbitrarily oriented in space

At the end of this section, we present numerical results for the spin polarization when the exchange field is oriented arbitrarily in space. These results are presented for a fixed chemical potential, fixed Rashba coupling constant, and definite magnitude of the exchange field. In such a case, the

vertex correction may only change the result by a constant factor, and therefore we plot the thermal spin polarizability in the bare bubble approximation (note that we also keep Γ small enough as to assume that we are in the quasiballistic limit). All three components of the spin polarization are shown in Fig. 4. The right column presents cross-sections of the density plots in the left panel, which correspond to an exchange field oriented in some specific planes. The density plots indicate the orientation of the exchange field where the spin polarization is maximal. This result is of importance for the magnetic dynamics induced by a spin torque due the spin polarization. Such a torque is created by the exchange coupling of the thermally induced spin polarization and magnetization. Since the induced spin polarization generally depends on the orientation of the exchange field, the torque contains a fieldlike and a dampinglike component.

V. MOTT RELATION FOR THERMALLY INDUCED MAGNETIZATION

For the kinetic coefficients describing the transport due to an electric field and a temperature gradient, it is possible to define the Mott relations. Generally, the Mott formula relates the derivative of the zero-temperature electric conductivity with the low temperature thermal conductivity. Other Mottlike relations have been presented recently for electrically and thermally induced spin transfer torques [44] and for electrically and thermally induced electric polarization [45]. However, such relations are not fundamental ones. It is well known that the Wiedemann-Franz law and Mott relations are satisfied for simple models, such as noninteracting electrons with parabolic bands [46,47]. More precisely, for finite systems where the strong energy dependence around the chemical potential does not allow for the Sommerfeld expansion or for strongly interacting systems, the Mott-like relations might be violated, see for instance Refs. [48-51] as well as the review [52] and references therein.

For spin-orbit driven phenomena, where the nonzero Berry curvature has a significant impact on the spin and transport properties, the Mott relation also might not be satisfied. The current section aims at combining the thermally induced spin polarizability with the electrically induced one (derived previously within the same formalism). We discuss the Mott-like formula for these two quantities.

In principle, the nonequilibrium spin polarization does not contribute to the entropy generation and does not behave like a kinetic coefficient. Thus, let us check if a proportionality between the derivative of the electrically induced spin polarization with respect to the chemical potential and the low-temperature thermally induced spin polarization exists. Defining in a standard way [47] the forces: $e\mathbf{E}$ and $-\nabla T/T$, we can write

$$S_{\alpha} = L_{\alpha\beta}^{(3)} e E_{\beta} + L_{\alpha\beta}^{(4)} \left(-\frac{\nabla_{\beta} T}{T} \right), \tag{65}$$

with $L_{\alpha\beta}^{(3)} = \chi_{\alpha}^{(E_{\beta})}$ and $L_{\alpha\beta}^{(4)} = -\chi_{\alpha}^{(\nabla_{\beta}T)}$. Here, $\chi_{\alpha}^{(E_{\beta})}$ is the electric field spin polarizability, while $\chi_{\alpha}^{(\nabla_{\beta}T)}$ is the thermal spin polarizability calculated in this paper. If the coefficients



FIG. 5. Comparison of the *y* component of thermally induced spin polarizability and the derivative of the electrically induced spin polarizability. The electrically induced spin polarizability is also plotted.

 $L_{\alpha\beta}^{(3,4)}$ satisfy the Mott relation we expect that

$$\chi_{\alpha}^{(\nabla_{\beta}T)} = -\frac{\pi^2}{3} (k_B T)^2 \partial_{\mu} \chi_{\alpha}^{(E_{\beta})}.$$
 (66)

For the nonmagnetic Rashba two-dimensional gas, the Edelstein formula does not depend on chemical potential

$$S_y^E = e E_x \frac{m\alpha}{2\pi\hbar^2} \tau, \tag{67}$$

and $\partial_{\mu}S_{y}^{E} = 0$. Accordingly, one can expect that the corresponding thermally induced spin polarization should be equal to zero. Equation (67) corresponds to Eq. (19). Indeed, this expression gives zero in the limit $\Gamma \rightarrow 0$.

For a nonmagnetic system as well as for a system with an exchange field normal to the plane of 2DEG, we compare the *x* and *y* components of the thermally induced spin polarization obtained from Eqs. (47) and (48) with the spin polarization induced by an electric field, which we obtained in one of our earlier works [42]. Figure 5 presents the electrically induced polarizability, $\chi_{x,y}^{(E)} \equiv S_{x,y}^{(E)}/eE_x$ (solid blue line) and its numerical derivative, normalized to the prefactor on the right side of Eq. (66) (dashed green line). Such normalized function overlaps very well with the thermally induced polarizability, $\chi_y^{(\nabla T)}$ (represented by solid red line). Note, the relaxation rate Γ is small and satisfies the relation $\Gamma \ll (2\zeta) \ll \mu$. Thus, the *y* components of the thermally and the electrically induced polarizations satisfy the Mott relation quite well, both in the nonmagnetic [Fig. 5(a)] and the magnetic [Figs. 5(b) and 5(d)] cases.

However, the Mott relation is not fulfilled for the x component of the thermally and electrically induced polarization. This is not surprising considering the fact that the x component of the polarization appears as a consequence of the two interactions: the spin-orbit interaction (here of the Rashba type), which mixes states for different subbands, and the exchange coupling, which breaks the time-reversal symmetry and leads to a nonzero Berry curvature. Both the x component of the thermally and electrically induced nonequilibrium polarization are determined by this topological term. Consequently, the states from the Fermi see are responsible for the effects. This is opposite to the case of the *y* components, where they are determined by the states at the Fermi level and, therefore, in the limit of small Γ , the Mott relation is fulfilled. Physically, one cannot expect a Mott-type relation when the spin polarizations are due to Berry curvature as there is no relation between derivative at the Fermi level and contribution from the whole band. Thus, the condition for the existence of the Mott relation between the field-induced and the thermally induced spin polarizations is the absence of the topological terms due to the Berry curvature. This condition may be formulated as (see Appendix **B**):

$$\operatorname{Tr} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \langle \sigma_{\alpha} \left(G_{\mathbf{k}}^{R}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{R}(\varepsilon) + G_{\mathbf{k}}^{A}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon) \right) \rangle = 0.$$
(68)

VI. SUMMARY AND CONCLUSIONS

We analyzed the spin polarization driven by a temperature gradient in a magnetized 2DEG with Rashba spin-orbit interaction. The limit of a nonmagnetic 2DEG has also been studied in detail. This limit was already studied earlier [12], but some approximations concerning the limit of small Rashba parameter turned out not to be adequate. Therefore, we have reconsidered this limit here in more detail and obtained results that properly describe the temperature dependence of the spin polarization.

For a magnetized 2DEG, we calculated the spin polarization for an arbitrary orientation of the exchange field, when all three components of the spin polarization can be nonzero. Such a general situation is important from the point of view of magnetic dynamics. Since the spin polarization leads to a spin torque exerted on the magnetization, the results can be useful when considering magnetic dynamics driven by an external thermal gradient. The torque due to the spin polarization can be presented generally as a sum of a fieldlike and a damping/antidamping term similarly, as in the spin-orbit torques driven by an external electric field or the spin transfer torques driven by an electric field in spin valves.

We note that the physical origin of the spin polarization due to a thermal gradient is different from that of the spin polarization driven by an external electric field. In the former case, the spin polarization is driven by a statistical force, while in the latter case this is an electrical force. As evidenced by the numerical calculations, the spin polarization induced by a temperature gradient reveals a peak whose maximum is around the band edge of the lower Rashba subband, where the asymmetry between the subbands generated by the Rashba coupling is largest. We find that the electrically induced and the thermally induced spin polarizations obey the Mott relation in a nonmagnetic 2DEG as well as in the magnetic system but in the latter case only for the spin polarization normal to the electric field and the thermal gradient. The components along the driving forces in a magnetic system do not obey this relation. This is because this component is mainly due to the Berry curvature of the electronic bands formed by the spin-orbit and the exchange interactions.

Finally, we would like to point out that the thermally induced spin polarization discussed here is different from the spin polarization due to the spin current in a magnetic system without a spin-orbit coupling (spin Seebeck effect) [53,54]. In the case of a spin Seebeck effect, the spin polarization appears as a spin accumulation in nanoscale systems. Moreover, the induced spin is oriented along the magnetic moment of the system, and therefore does not generate a torque on the magnetic moment. This is in the contrast to the thermally induced polarization discussed here. Due to the spin-orbit interaction, the leading term describing the nonequilibrium spin polarization is oriented perpendicularly to the magnetization and generates a torque.

ACKNOWLEDGMENTS

This work was supported by the Polish Ministry of Science and Higher Education through a research project Iuventus Plus in years 2015-2017 (Project No. 0083/IP3/2015/73) and the Deutsche Forschungsgemeinschaft, DFG (No. SFB 762, and SFB TRR 227). A.D. acknowledges the support from the Foundation for Polish Science (FNP). V.D. acknowledges support from the National Science Center in Poland under Grant No. DEC-2012/06/M/ST3/00042.

APPENDIX A: KINETIC COEFFICIENTS AND ENTROPY GENERATION

Macroscopic equations for electric current **j**, heat flux $\tilde{\mathbf{q}} = \mathbf{q} - \varphi \mathbf{j}$ (with **q** being the energy flux and $\varphi = \mu/e$) and spin polarization **S** induced by the temperature gradient and electric field **E** in the 2D system with Rashba spin-orbit coupling and magnetization **M** along axis *z* can be written as

$$\mathbf{j} = \sigma \mathbf{E} - \alpha_S \nabla T + \sigma_H \mathbf{M} \times \mathbf{E} + \alpha_N \mathbf{M} \times \nabla T, \quad (A1)$$

$$\tilde{\mathbf{q}} = \beta \mathbf{E} - \kappa \nabla T + \alpha_q \, \mathbf{M} \times \mathbf{E} + \alpha_R \, \mathbf{M} \times \nabla T, \quad (A2)$$

$$\mathbf{S} = \gamma \mathbf{M} + \alpha_E \, \mathbf{n} \times \mathbf{E} + \alpha_{ET} \, \mathbf{n} \times \nabla T + \alpha_C \, \mathbf{n} \times (\mathbf{M} \times \mathbf{E}) + \alpha_{CT} \, \mathbf{n} \times (\mathbf{M} \times \nabla T), \tag{A3}$$

where **n** is the Rashba SO vector perpendicular to the plane, σ is the conductance, α_S is the Seebeck coefficient, σ_H is the anomalous Hall conductance, α_N is the Nernst coefficient, β is the thermoelectric coefficient, κ is heat conductance, α_E is coefficient of electrically induced magnetization, etc. These phenomenological equations take into account that **j**, **E**, ∇T , **n** are polar vectors, whereas **M** and **S** are axial vectors (pseudovectors). These equations in components, assuming

that the magnetization **M** is along axis *z*:

$$j_x = \sigma E_x - \alpha_S \nabla_x T - \sigma_H M E_y - \alpha_N M \nabla_y T, \qquad (A4)$$

$$j_{y} = \sigma E_{y} - \alpha_{S} \nabla_{y} T + \sigma_{H} M E_{x} + \alpha_{N} M \nabla_{x} T, \qquad (A5)$$

$$\tilde{q}_x = \beta E_x - \kappa \nabla_x T - \alpha_q M E_y - \alpha_R M \nabla_y T, \qquad (A6)$$

$$\tilde{q}_y = \beta E_y - \kappa \nabla_y T + \alpha_q M E_x + \alpha_R M \nabla_x T, \qquad (A7)$$

$$S_x = -\alpha_E E_y - \alpha_{ET} \nabla_y T - \alpha_C M E_x - \alpha_{CT} M \nabla_x T,$$
 (A8)

$$S_y = \alpha_E E_x + \alpha_{ET} \nabla_x T - \alpha_C M E_y - \alpha_{CT} M \nabla_y T.$$
 (A9)

The generation of entropy in a small area per unit time is $\delta S = \delta Q/T$, where δQ is the generated heat. Then we get

$$\frac{\partial S}{\partial t} = -\int d^2 \mathbf{r} \, \frac{\nabla \cdot \mathbf{q}}{T} = \int d^2 \mathbf{r} \, \frac{\mathbf{j} \cdot \mathbf{E} - \nabla \cdot \mathbf{\tilde{q}}}{T}$$
$$= \int d^2 \mathbf{r} \left(\frac{\mathbf{j} \cdot \mathbf{E}}{T} - \frac{\mathbf{\tilde{q}} \cdot \nabla T}{T^2} \right), \tag{A10}$$

where integration is over the area of 2D system. In accordance with the Onsager principle,

$$\frac{\partial S}{\partial t} = -\int d^2 \mathbf{r} \ X_a \ \frac{\partial x_a}{\partial t}.$$
 (A11)

We can choose $\dot{x}_1 = j_x$, $\dot{x}_2 = j_y$, $\dot{x}_3 = \tilde{q}_x$, $\dot{x}_4 = \tilde{q}_y$. Then comparing Eqs. (A10) and (A11), we get $X_1 = -\frac{E_x}{T}$, $X_2 = -\frac{E_y}{T}$, $X_3 = \frac{\nabla_x T}{T^2}$, $X_4 = \frac{\nabla_y T}{T^2}$. On the other hand, the kinetic coefficients γ_{ab} should be defined from the Onsager relation:

$$\frac{\partial x_a}{\partial t} = -\gamma_{ab} X_b. \tag{A12}$$

Correspondingly, we have to rewrite the set of Eqs. (A4)–(A9) in a matrix form

$$\begin{pmatrix} j_x \\ j_y \\ \tilde{q}_x \\ \tilde{q}_y \end{pmatrix} = \begin{pmatrix} -\sigma T & \sigma_H M T & -\alpha_S T^2 & -\alpha_N M T^2 \\ -\sigma_H M T & -\sigma T & \alpha_N M T^2 & -\alpha_S T^2 \\ -\beta T & \alpha_q M T & -\kappa T^2 & -\alpha_R M T^2 \\ -\alpha_q M T & -\beta T & \alpha_R M T^2 & -\kappa T^2 \end{pmatrix} \times \begin{pmatrix} -\frac{E_x}{T} \\ -\frac{E_y}{T} \\ \frac{\nabla_x T}{T^2} \\ \frac{\nabla_y T}{T^2} \end{pmatrix}.$$
 (A13)

Since the symmetry of kinetic coefficients is expressed by relation

$$\gamma_{ab}(M) = \gamma_{ba}(-M), \tag{A14}$$

we obtain

$$\beta = \alpha_S T, \tag{A15}$$

$$\alpha_q = -\alpha_N T. \tag{A16}$$

The other symmetry relations are fulfilled automatically.

Let us assume that $j_y = 0$, $E_x = 0$ and $\nabla_y T = 0$. Then, from Eq. (A5), we find

$$E_y = -\frac{\alpha_N M}{\sigma} \nabla_x T. \tag{A17}$$

Substituting Eq. (A17) into Eqs. (A4)–(A9), we obtain

$$j_x = -\left(\alpha_S - \frac{\sigma_H \alpha_N M^2}{\sigma}\right) \nabla_x T, \qquad (A18)$$

$$\tilde{q}_x = -\left(\kappa - \frac{\alpha_q \alpha_N M^2}{\sigma}\right) \nabla_x T,$$
 (A19)

$$\tilde{q}_y = \left(\alpha_R - \frac{\beta \alpha_N}{\sigma}\right) M \nabla_x T, \qquad (A20)$$

$$S_x = -\left(\alpha_{CT} + \frac{\alpha_E \alpha_N}{\sigma}\right) M \nabla_x T, \qquad (A21)$$

$$S_y = \left(\alpha_{ET} + \frac{\alpha_C \alpha_N M^2}{\sigma}\right) \nabla_x T,$$
 (A22)

which demonstrates the effect of anomalous Hall and Nerst effects on the Seebeck current, the heat flux and the spin polarization.

The entropy generation rate is

$$\frac{\partial S}{\partial t} = \int d^2 \mathbf{r} \, \frac{(\kappa \sigma - \alpha_q \alpha_N M^2) (\nabla_x T)^2}{\sigma T^2}. \tag{A23}$$

Thus, the entropy generation is not affected by spin polarization S but is determined by the heat flux along axis x.

In the limit of $\nabla_x T/T \to 0$ and $T \to 0$, from Eq. (A23) follows that $\partial S/\partial t \to 0$ if $\kappa \to 0$ and $\sigma \to \text{const}$ (due to the Wiedemann-Franz law). It does not automatically mean that the corresponding coefficients for S_x and S_y are zero in this limit (even if $\alpha_N \to 0$) because α_{CT} and/or α_{CE} can be finite at $T \to 0$, and it does not contradict to the thermodynamics.

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APPENDIX B: CONDITION FOR THE MOTT RELATION

Here we discuss the general conditions when the Mott Relation is satisfied. In the general case, the electric-field induced spin polarization can be written as follows:

$$S_{\alpha}^{E}(\omega) = \frac{\hbar}{\omega} \operatorname{Tr} \int \frac{d\varepsilon}{2\pi} f_{\varepsilon} \langle \hat{s}_{\alpha} \left[G_{\mathbf{k}}^{R}(\varepsilon + \omega) \hat{v}_{x} \left(G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \right) + \left(G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon) \right) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon - \omega) \right] \rangle, \tag{B1}$$

where the triangle bracket means an averaging over impurities. In the dc limit, we find

$$S_{\alpha}^{E} = \hbar \operatorname{Tr} \int \frac{d\varepsilon}{2\pi} \left\langle \hat{s}_{\alpha} \Big[f'(\varepsilon) G_{\mathbf{k}}^{R}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon) - f(\varepsilon) \Big[G_{\mathbf{k}}^{R}(\varepsilon) \Big]^{2} \hat{v}_{x} \right. \\ \left. \times G_{\mathbf{k}}^{R}(\varepsilon) - f(\varepsilon) G_{\mathbf{k}}^{A}(\varepsilon) \hat{v}_{x} \Big[G_{\mathbf{k}}^{A}(\varepsilon) \Big]^{2} \Big] \right\rangle.$$
(B2)

In turn, the thermally induced spin polarization is given by the expression

$$S_{\alpha}^{\nabla T}(\omega) = \frac{\hbar}{2\omega} \operatorname{Tr} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \langle \hat{s}_{\alpha} [G_{\mathbf{k}}^{R}(\varepsilon + \omega)[\hat{H} - \mu\sigma_{0}, \hat{v}_{x}]_{+} \\ \times (G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon)) + (G_{\mathbf{k}}^{R}(\varepsilon) - G_{\mathbf{k}}^{A}(\varepsilon)) \\ \times [\hat{H} - \mu\sigma_{0}, \hat{v}_{x}]_{+} G_{\mathbf{k}}^{A}(\varepsilon - \omega)] \rangle.$$
(B3)

This equation in the dc limit leads to the expression

$$S_{\alpha}^{\nabla T} = \hbar \operatorname{Tr} \int \frac{d\varepsilon}{2\pi} \left\langle \hat{s}_{\alpha}(\varepsilon - \mu) \left[- f(\varepsilon) \left[G_{\mathbf{k}}^{R}(\varepsilon) \right]^{2} \hat{v}_{x} G_{\mathbf{k}}^{R}(\varepsilon) \right. \right. \\ \left. + f'(\varepsilon) G_{\mathbf{k}}^{R}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon) - f_{\mathbf{k}}(\varepsilon) G_{\mathbf{k}}^{A}(\varepsilon) \hat{v}_{x} \left[G_{\mathbf{k}}^{A}(\varepsilon) \right]^{2} \right] \\ \left. + \frac{1}{2} \hat{s}_{\alpha} f(\varepsilon) \left[G_{\mathbf{k}}^{R}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{R}(\varepsilon) + G_{\mathbf{k}}^{A}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon) \right] \right\rangle.$$

$$(B4)$$

Thus, the Mott relation is fulfilled if

. .

$$\operatorname{Tr} \int \frac{d\varepsilon}{2\pi} f(\varepsilon) \langle \sigma_{\alpha} \left(G_{\mathbf{k}}^{R}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{R}(\varepsilon) + G_{\mathbf{k}}^{A}(\varepsilon) \hat{v}_{x} G_{\mathbf{k}}^{A}(\varepsilon) \right) \rangle = 0.$$
(B5)

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