Nonlinear spin-current generation in quantum wells with arbitrary Rashba-Dresselhaus spin-orbit interactions

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The problem of the nonlinear spin-currents generated by an electric field $\mathbf{E}$ and a temperature gradient ∇T in spin-orbit coupled systems is revisited in a different formalism. Here, the second-order correction to the particle distribution function $\delta f^{(2)}$ is derived in a semiclassical approximation that takes into account the local change in the equilibrium distribution function induced by the external fields. Our approach departs significantly from the present theory, where $\delta f^{(2)}$ is written as an iterative solution to the Boltzmann transport equation in the relaxation-time approximation. As we show, such an expression does not actually satisfy the collision term of the equation, and therefore it is not self-consistent. We apply our formalism to the case of a quantum well with arbitrary values of the linear Rashba α and Dresselhaus β interactions. For the whole range of α versus β values, we obtain analytic results for all the spin currents that can be driven in the system, proportional with $\mathbf{E}^2$, ∇T^2, or with $\mathbf{E} \cdot \nabla T$. The magnitude of these currents is smaller than previously anticipated.

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I. INTRODUCTION

Studied intensively for the past decade, spin-orbit (SO) coupled systems continue to provide an interesting exploration ground for theoretical and experimental investigations focused on detecting phenomena that can lead to the establishment of a spin-dependent transport paradigm for applications [1,2]. Of all systems endowed with some form of spin-orbit interaction, two-dimensional III-V semiconductor quantum wells with inversion asymmetry occupy a preeminent spot, given their well-understood behavior as normal Fermi systems, which, coupled with the high degree of electric control over the SO parameters, makes them suitable for a large range of experiments [3–9]. There, the spin-orbit interaction is described by the linear coupling between the spin and momentum with strength α for the Rashba term, which originates in the inversion asymmetry of the well [10], and with strength β for the Dresselhaus term, which originates in the inversion asymmetry of the crystal [11]. Since the two terms rotate the spin in opposite directions, their simultaneous consideration in theoretical investigations is somewhat challenging, and often solutions are given only in numerical formalisms.

The search for the realization of stable spin currents in two-dimensional systems has received an important impetus from the predicted nonlinear generation of such currents in anisotropic Fermi pockets that relied on using the second-order correction to the distribution function induced by the electric field or temperature gradient, $\delta f^{(2)}$ [12]. The idea behind this approach exploits the even parity in the momentum space of $\delta f^{(2)}$ written as an iterative solution of the Boltzmann transport equation (BTE) in the relaxation-time approximation, which is juxtaposed on the anisotropy of the single-particle energy spectrum to create a nonzero differential valley or spin-current effect. In the presence of an electric field $\mathbf{E}$ and a temperature gradient ∇T, spin and charge currents proportional to $\mathbf{E}^2$ and $(\nabla T)^2$ were calculated to have, in both cases, significant values, thus heralding a new paradigm for experimental realization.

More recently, the same computational algorithm was applied to the case of a semiconductor quantum well with Rashba and Dresselhaus spin-orbit interaction in Ref. [13], where spin currents quadratic in the applied electric field were evaluated. Analytic expressions were derived when only one interaction was present, either $\alpha = 0$ or $\beta = 0$, while numerical results were obtained for the case of both couplings being considered. Thus, it was found that pure spin currents, whose amplitude is proportional with α or β, are driven simultaneously along parallel and perpendicular directions on the electric field. In each case, the spin polarization is perpendicular to the direction of propagation. The calculated magnitude of the parallel and perpendicular currents is different, with the current along the direction of the electric field about five times larger, but in both cases it was significant enough to exceed the values obtained by other electric means. A numerical study of the case $\alpha \neq 0$ and $\beta \neq 0$ indicated that both currents disappear in the limit $\alpha = \beta$.

In this paper, we reformulate the theory of nonlinear spin currents by using a different expression for $\delta f^{(2)}$. This is necessary since, as we demonstrate below, a second-order distribution function cannot be derived iteratively in the relaxation-time approximation as it does not satisfy self-consistently the collision term of the Boltzmann transport equation. Instead, we calculate $\delta f^{(2)}$ from a power expansion of the Fermi distribution function written in a semiclassical approximation for a local energy configuration that reflects the change in the electron energy in the presence of the electric field and the change in the Boltzmann factor in the presence of a temperature gradient. The spatial validity of this approximation is established by the average distance between two successive collisions, which is proportional to the relaxation time. This limitation is imposed by the requirement that the first-order correction to the distribution function $\delta f^{(1)}$ derived in this way coincides with the solution of the Boltzmann equation linear in the external fields.

Our nonlinear transport formalism is applied to the case of a two-dimensional electron gas in a quantum well with Rashba and Dresselhaus spin-orbit interactions. Analytic expressions for the nonlinear spin currents are calculated for arbitrary values of the Rashba and Dresselhaus coupling constants in the presence of an electric field and a temperature gradient. The spin polarization of the currents is parallel or perpendicular to the direction of propagation depending on the geometric distribution of the applied perturbations. Their amplitude is proportional to the spin-orbit coupling constants and cancels in the limit $\alpha = \beta$ regardless of the directions of the applied fields and propagation.

II. SECOND-ORDER DISTRIBUTION FUNCTION

We consider a simple two-dimensional Fermi system described by a single-particle Hamiltonian H whose eigenvalues $\epsilon_{\mathbf{p}}$ are functions of the momentum $\mathbf{p}$. Other quantum numbers, such as spin (or valley index), might be present, but since they are not relevant at this point, they will not be explicitly declared. In thermodynamic equilibrium, the statistical occupancy of a single-particle state is established by the Fermi distribution function at temperature T, $f^0_{\mathbf{p}} = [1 + \exp\frac{\epsilon_{\mathbf{p}}-\epsilon_F}{k_BT}]^{-1}$, where ϵ_F is the Fermi energy.

In the presence of a time-independent perturbation, $f(\mathbf{p},\mathbf{r})$, function of position $\mathbf{r}$ and momentum $\mathbf{p}$, describes the particle distribution and satisfies the general Boltzmann transport equation (BTE),

$$\left[\frac{\partial f(\mathbf{p},\mathbf{r})}{\partial t}\right] = \left[\frac{\partial f(\mathbf{p},\mathbf{r})}{\partial t}\right]_{\text{coll.}}. \tag{1}$$

This equality expresses the conservation of the number of particles in a volume in the phase space, as particles leave the trajectory prescribed by Hamilton's equations only as a result of collisions. Introducing $\delta f_{\mathbf{p}}(\mathbf{r})$ as the deviation equilibrium of the distribution function, a solution of the BTE is

$$f(\mathbf{r},\mathbf{p}) = f^0_{\mathbf{p}} + \delta f_{\mathbf{p}}(\mathbf{r}). \tag{2}$$

Henceforth, the explicit dependence on $\mathbf{r}$ of $\delta f_{\mathbf{p}}(\mathbf{r})$ will not be declared, considering that it does not play a role in the collision integral, the central part of our analysis. With this, the collision term can be written as

$$\begin{aligned}\left[\frac{\partial f(\mathbf{r},\mathbf{p})}{\partial t}\right]_{\text{coll.}} &= -\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}[f_{\mathbf{p}}(1-f_{\mathbf{p}'}) - f_{\mathbf{p}'}(1-f_{\mathbf{p}})]\\ &= -\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}(\delta f_{\mathbf{p}} - \delta f_{\mathbf{p}'}),\end{aligned} \tag{3}$$

where $P_{\mathbf{p},\mathbf{p}'}$ is the probability of scattering between states of momenta $\mathbf{p}$ and $\mathbf{p}'$. For a scattering matrix element $V_{\mathbf{p},\mathbf{p}'}(\theta_{\mathbf{pp}'})$, which depends at most on the angle between the initial and final momentum states $\theta_{\mathbf{p},\mathbf{p}'}$, the Fermi golden rule generates

$$P_{\mathbf{p},\mathbf{p}'} = \frac{2\pi}{\hbar}|V_{\mathbf{pp}'}(\theta_{\mathbf{pp}'})|^2\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}). \tag{4}$$

When Eq. (1) is written for the deviation from equilibrium of the distribution function in all orders in the external fields $\delta f^{(n)}_{\mathbf{p}}$, an additional perturbation is introduced via $\dot{\mathbf{p}}$ and $\dot{\mathbf{r}}$ from Hamilton's equations of motion. Therefore, the general iterative equation satisfied is

$$\begin{aligned}&\dot{\mathbf{p}}\cdot\nabla_{\mathbf{p}}\delta f^{(n-1)}_{\mathbf{p}} + \dot{\mathbf{r}}\cdot\nabla_{\mathbf{r}}\delta f^{(n-1)}_{\mathbf{p}}\\ &\quad= -\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\big(\delta f^{(n)}_{\mathbf{p}} - \delta f^{(n)}_{\mathbf{p}'}\big), \quad n \geqslant 1.\end{aligned} \tag{5}$$

In equilibrium, of course, $(\frac{\partial f^0_{\mathbf{p}}}{\partial t})_{\text{coll.}} = 0$.

A. Present theory

The present theory of nonlinear spin and charge currents discussed in Refs. [12,13] is based on deriving $\delta f^{(2)}_{\mathbf{p}}$, the distribution function that is quadratic in the applied fields, by approximating the collision term in Eq. (5) for $n = 2$ "in the relaxation time approximation." Thus, generalizing for the nth order,

$$\dot{\mathbf{p}}\cdot\nabla_{\mathbf{p}}\delta f^{(n-1)}_{\mathbf{p}} + \dot{\mathbf{r}}\cdot\nabla_{\mathbf{r}}\delta f^{(n-1)}_{\mathbf{p}} = -\frac{\delta f^{(n)}_{\mathbf{p}}}{\tau} \quad (n \geqslant 1). \tag{6}$$

τ is the energy-independent relaxation time, the average time between two consecutive collisions.

In the following considerations, we assume for simplicity that only an in-plane electric field is applied. Then, the first-order correction to the distribution function $\delta f^{(1)}_{\mathbf{p}}$ is obtained from Eq. (6) when $n = 1$ and $\dot{\mathbf{p}} = -e\mathbf{E}$, in the relaxation-time approximation as

$$\delta f^{(1)}_{\mathbf{p}} = e\tau E\frac{\partial f^0_{\mathbf{p}}}{\partial p_\parallel}, \tag{7}$$

where $p_\parallel$ is the projection of the electron momentum along the direction of the electric field ($p_\perp$ is the component of the linear momentum perpendicular to the field). This is simply the well-known linear textbook solution for the BTE.

For $n = 2$, the second-order correction to the particle distribution function follows immediately from (6) and (7) as

$$\delta f^{(2)}_{\mathbf{p}} = (e\tau E)^2\frac{\partial^2 f^0_{\mathbf{p}}}{\partial p^2_\parallel}, \tag{8}$$

while the nth-order generalization is [13]

$$\delta f^{n}_{\mathbf{p}} = (e\tau E)^n\frac{\partial^n f^0_{\mathbf{p}}}{\partial p^n_\parallel}. \tag{9}$$

Using (8), nonlinear currents are obtained by summing a generic (spin or valley-charge) velocity operator matrix element $\tilde{v}_{\mathbf{p}}$ multiplied by $\delta f^{(2)}_{\mathbf{p}}$ over the two-dimensional momentum space. Symmetry considerations require that a nonzero result is obtained only if the two terms have the same parity, even in the momentum. Thus,

$$\delta\mathbf{j} = \sum_{\mathbf{p}}\tilde{\mathbf{v}}_{\mathbf{p}}\delta f^{(2)}_{\mathbf{p}} = (e\tau E)^2\sum_{\mathbf{p}}\tilde{\mathbf{v}}_{\mathbf{p}}\frac{\partial^2 f^0_{\mathbf{p}}}{\partial p^2_\parallel}. \tag{10}$$

When implemented for a 2D electron system with either Rashba or Dresselhaus interactions, this algorithm leads to analytic expressions predicting the existence of spin currents whose magnitude is proportional with α or β, respectively. Numerical results are obtained when both spin-orbit couplings are present. In the limit of $\alpha = \beta$, when the two spin-orbit interactions are equal, no spin currents are found [13].

As we demonstrate below, however, using Eq. (6) in deriving a second-order correction to the particle density distribution function is not appropriate since, for $n \geqslant 2$, the collision term in Eq. (5) *cannot be* approximated in the relaxation-time approximation,

$$\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\big(\delta f_{\mathbf{p}}^{(n)} - \delta f_{\mathbf{p}'}^{(n)}\big) \neq \frac{\delta f_{\mathbf{p}}^{(n)}}{\tau}, \quad n \geqslant 2. \tag{11}$$

B. The relaxation-time approximation to the Boltzmann equation

When Eq. (5) is written for $n = 1$, the first-order correction to the equilibrium particle distribution function satisfies

$$e\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}} = \sum_{\mathbf{p}'} P_{\mathbf{p}\mathbf{p}'}\big[\delta f_{\mathbf{p}}^{(1)} - \delta f_{\mathbf{p}'}^{(1)}\big], \tag{12}$$

where $\mathbf{v}_{\mathbf{p}} = \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}$ is the velocity of the particle.

Solving Eq. (12) for $\delta f_{\mathbf{p}}^{(1)}$ starts by proposing a self-consistent solution of the form

$$\delta f_{\mathbf{p}}^{(1)} = C(\epsilon_{\mathbf{p}})(e\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}}, \tag{13}$$

where $C(\epsilon_{\mathbf{p}})$ is a constant, at most dependent on energy. With this choice, the right-hand side of Eq. (12) becomes

$$\begin{aligned}
&\sum_{\mathbf{p}'} P_{\mathbf{p}\mathbf{p}'}\big(\delta f_{\mathbf{p}}^{(1)} - \delta f_{\mathbf{p}'}^{(1)}\big)\\
&= \frac{2\pi}{\hbar}\sum_{\mathbf{p}'} |V(\theta_{\mathbf{p},\mathbf{p}'})|^2\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'})\big(\delta f_{\mathbf{p}}^{(1)} - \delta f_{\mathbf{p}'}^{(1)}\big)\\
&= eC(\epsilon_{\mathbf{p}})E v_{\mathbf{p}}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}}\frac{\nu_0}{\hbar}\int_0^{2\pi} d\theta_{\mathbf{p},\mathbf{p}'}|V(\theta_{\mathbf{p},\mathbf{p}'})|^2\\
&\quad\times[\cos\theta_{\mathbf{p},\mathbf{E}} - \cos\theta_{\mathbf{p}',\mathbf{E}}]\\
&= \delta f_{\mathbf{p}}^{(1)}\frac{\nu_0}{\hbar}\int_0^{2\pi} d\theta_{\mathbf{p},\mathbf{p}'}|V(\theta_{\mathbf{p},\mathbf{p}'})|^2(1 - \cos\theta_{\mathbf{p},\mathbf{p}'})\\
&= \frac{\delta f_{\mathbf{p}}^{(1)}}{\tau}.
\end{aligned} \tag{14}$$

The end result is possible because the scattering matrix element $|V_{\mathbf{p},\mathbf{p}'}|^2$ is an even function of $\theta_{\mathbf{p},\mathbf{p}'}$ implying that the odd part of $\cos\theta_{\mathbf{p}',\mathbf{E}} = \cos(\theta_{\mathbf{p},\mathbf{E}} + \theta_{\mathbf{p},\mathbf{p}'})$ does not contribute to the angular integral. Therefore $C(\epsilon_{\mathbf{p}}) = \tau$, the electron relaxation time, same as in Eq. (6), given by

$$\frac{\hbar}{\tau} = \nu_0\int |V_{\mathbf{p},\mathbf{p}'}|^2(1 - \cos\theta_{\mathbf{p}\mathbf{p}'})d\theta_{\mathbf{p}\mathbf{p}'}, \tag{15}$$

with ν_0 the density of states at the Fermi surface. The final form of $\delta f_{\mathbf{p}}^{(1)}$ is also obtained in a quantum-mechanical formalism that evaluates the conductivity as a linear-response function to an electric field. It is equivalent to the renormalization of the electron velocity (current vertex renormalization) on account of impurity-mediated scattering [14].

It is important to accentuate the idea that the transport time τ appears in the expression of $\delta f_{\mathbf{p}}^{(1)}$ precisely because it was assumed that $\delta f_{\mathbf{p}}^{(1)}$ is of the form (13) when the collision term in the BTE was calculated.

When one solves Eq. (5) for $n = 2$, the above procedure has to be repeated. Therefore, a second-order solution should be of the form

$$\delta f_{\mathbf{p}}^{(2)} = C(\epsilon_{\mathbf{p}})(e\mathbf{E}\cdot\nabla_{\mathbf{p}})\delta f_{\mathbf{p}}^{1} = C(\epsilon_{\mathbf{p}})\tau(e\mathbf{E}\cdot\nabla_{\mathbf{p}})^2 f_{\mathbf{p}}^{0}, \tag{16}$$

where as before $C(\epsilon_{\mathbf{p}})$ is a constant, at most dependent on the energy. With this choice, the collision integral in Eq. (5) becomes

$$\begin{aligned}
&\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\big(\delta f_{\mathbf{p}}^{(2)} - \delta f_{\mathbf{p}'}^{(2)}\big)\\
&= C(\epsilon_{\mathbf{p}})\tau(eE)^2\frac{\nu_0}{\hbar}\int_0^{2\pi} d\theta_{\mathbf{p}'}|V(\theta_{\mathbf{p},\mathbf{p}'})|^2\left[\frac{\partial^2 f_{\mathbf{p}}^{0}}{\partial p_\parallel^2} - \frac{\partial^2 f_{\mathbf{p}}^{0}}{\partial (p')_\parallel^2}\right].
\end{aligned} \tag{17}$$

A straightforward calculation yields

$$\begin{aligned}
\frac{\partial^2 f_{\mathbf{p}}^{0}}{\partial p_\parallel^2} &= \frac{\partial}{\partial p_\parallel}\left(\frac{\partial \epsilon_{\mathbf{p}}}{\partial p_\parallel}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}}\right) = \frac{\partial^2 \epsilon_{\mathbf{p}}}{\partial p_\parallel^2}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}} + \left(\frac{\partial \epsilon_{\mathbf{p}}}{\partial p_\parallel}\right)^2\frac{\partial^2 f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}^2}\\
&= \frac{\partial^2 \epsilon_{\mathbf{p}}}{\partial p_\parallel^2}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}} - \frac{1}{k_B T}\left(\frac{\partial \epsilon_{\mathbf{p}}}{\partial p_\parallel}\right)^2\tanh\frac{\epsilon_{\mathbf{p}} - \epsilon_F}{2k_B T}\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}}.
\end{aligned} \tag{18}$$

When Eq. (18) is used to evaluate the collision integral, we obtain

$$\begin{aligned}
&\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\big(\delta f_{\mathbf{p}}^{(2)} - \delta f_{\mathbf{p}'}^{(2)}\big)\\
&= C(\epsilon_{\mathbf{p}})\tau(eE)^2\frac{\partial f_{\mathbf{p}}^{0}}{\partial \epsilon_{\mathbf{p}}}\frac{\nu_0}{\hbar}\left\{\int_0^{2\pi} d\theta_{\mathbf{p}'}|V(\theta_{\mathbf{p},\mathbf{p}'})|^2\right.\\
&\quad\times\left[\frac{\partial^2 \epsilon_{\mathbf{p}}}{\partial p_\parallel^2} - \frac{\partial^2 \epsilon_{\mathbf{p}'}}{\partial (p')_\parallel^2}\right] - v_{\mathbf{p}}^2\frac{1}{k_B T}\tanh\frac{\epsilon_{\mathbf{p}} - \epsilon_F}{2k_B T}\\
&\quad\times\left.\int_0^{2\pi} d\theta_{\mathbf{p}'}|V(\theta_{\mathbf{p},\mathbf{p}'})|^2(\cos^2\theta_{\mathbf{p},\mathbf{E}} - \cos^2\theta_{\mathbf{p}',\mathbf{E}})\right\}\\
&\neq \frac{\delta f_{\mathbf{p}}^{(2)}}{\tau},
\end{aligned} \tag{19}$$

where τ has to be the same as in Eq. (15).

Consequently, a second-order solution cannot be obtained in the "relaxation-time approximation" since it does not satisfy consistently the right-hand side of the BTE, i.e., the collision integral. Any other higher-order approximation cannot be obtained in this way, either. The gist of this argument is that in order for $\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\delta f_{\mathbf{p}'}^{(n)} \sim \delta f_{\mathbf{p}}^{(n)}$, $\delta f_{\mathbf{p}}^{(n)}$ has to have an angular dependence that is given exactly by $\mathbf{v}_{\mathbf{p}}\cdot\mathbf{E}$, which is true only in first order in the perturbative fields.

It is clear, therefore, that the generalization Eq. (9) is inaccurate as it neglects the second term of the collision integral, $\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\delta f_{\mathbf{p}'}^{(n)}$. In reality, this term is of the same order as $\sum_{\mathbf{p}'} P_{\mathbf{p},\mathbf{p}'}\delta f_{\mathbf{p}}^{(n)} = \delta f_{\mathbf{p}}^{(n)}/\tau$ (assuming isotropic scattering), so its disappearance is not justified.

C. The local approximation to the particle distribution function

Here we discuss a different algorithm that generates the second-order distribution function in a semiclassical approximation, based on the local perturbation of the single-particle distribution function induced by the external fields. The addition of an electrostatic potential $V(\mathbf{r}) = -\mathbf{E}\cdot\mathbf{r}$ modifies locally the electron energy to $\tilde{\epsilon}_{\mathbf{p}} = \epsilon_{\mathbf{p}} + e\mathbf{E}\cdot\mathbf{r}$, while a temperature gradient changes the Boltzmann factor to $1/k_B(T + \nabla T\cdot\mathbf{r})$. If these changes are weak compared with the Fermi energy, the electron distribution function is just the Fermi function written for the local energy and Boltzmann factor,

$$\tilde{f}_{\mathbf{p}}(\mathbf{r}) = \left\{1 + \exp\left[\frac{\epsilon_{\mathbf{p}} - \epsilon_F + e\mathbf{E}\cdot\mathbf{r}}{k_B(T + \nabla T\cdot\mathbf{r})}\right]\right\}^{-1}. \tag{20}$$

Equation (20) can be expanded in a series of terms proportional to powers of the electric field and the temperature gradient, respectively. When the linear terms are constrained to replicate the solution of the BTE, it is found that $\mathbf{r} = \mathbf{v}_{\mathbf{p}}\tau$, a result that establishes the spatial range of the approximation.

With this input, the expansion of the distribution function becomes

$$\begin{aligned}\tilde{f}_{\mathbf{p}} = f^0_{\mathbf{p}} &+ \left[(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}}) - (\epsilon_{\mathbf{p}} - \epsilon_F)\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)\right]\frac{\partial f^0_{\mathbf{p}}}{\partial\epsilon_{\mathbf{p}}}\\ &+ \frac{1}{2}\left\{\left[(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})^2 + (\epsilon_{\mathbf{p}} - \epsilon_F)^2\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)^2\right.\right.\\ &\left. - 2(\epsilon_{\mathbf{p}} - \epsilon_F)(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)\right]\frac{\partial^2 f^0_{\mathbf{p}}}{\partial\epsilon^2_{\mathbf{p}}}\\ &+ \left[2(\epsilon_{\mathbf{p}} - \epsilon_F)\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)^2 - 2(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})\right.\\ &\left.\left. \times\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)\right]\frac{\partial f^0_{\mathbf{p}}}{\partial\epsilon_{\mathbf{p}}}\right\}. \end{aligned} \tag{21}$$

Immediately, the second-order distribution function is therefore

$$\begin{aligned}\delta f^{(2)}_{\mathbf{p}} = \frac{1}{2}&\left\{\left[(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})^2 + (\epsilon_{\mathbf{p}} - \epsilon_F)^2\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)^2\right.\right.\\ &\left. - 2(\epsilon_{\mathbf{p}} - \epsilon_F)(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)\right]\frac{\partial^2 f^0_{\mathbf{p}}}{\partial\epsilon^2_{\mathbf{p}}}\\ &+ \left[2(\epsilon_{\mathbf{p}} - \epsilon_F)\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)^2 - 2(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})\right.\\ &\left.\left. \times\left(\tau\mathbf{v}_{\mathbf{p}}\cdot\frac{\nabla T}{T}\right)\right]\frac{\partial f^0_{\mathbf{p}}}{\partial\epsilon_{\mathbf{p}}}\right\}. \end{aligned} \tag{22}$$

Obtained in this way, $\delta f^{(2)}_{\mathbf{p}}$ is not required to satisfy the Boltzmann transport equation since its derivation is not associated with an evaluation of the collision integral. In the degenerate Fermi gas approximation, the only term in Eq. (21) that does not cancel is the one proportional to both electric field and temperature gradient. Evaluating the current integrals requires the Sommerfeld algorithm for all of the remaining cases.

Moreover, the nth-order deviation from equilibrium induced by an applied electric field is, in contrast with Eq. (9),

$$\delta f^n_{\mathbf{p}} = \frac{1}{n!}(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})^n\frac{\partial^n f^0_{\mathbf{p}}}{\partial\epsilon^n_{\mathbf{p}}}. \tag{23}$$

III. SPIN CURRENTS

Using the second-order distribution function derived above, we calculate the quadratic spin currents driven by an electric field and a temperature gradient in a quantum well with arbitrary Rashba and Dresselhaus interactions.

A. Single-particle Hamiltonian

We consider a 2D electron system in a [100] quantum well described in a system of reference with the $\hat{y}$ perpendicular on the plane. The $\hat{x}$-$\hat{z}$ in-plane axes are rotated by $\pi/4$ from the usual directions such that $x \parallel [110]$ and $z \parallel [1\bar{1}0]$ [15]. This choice of axes takes advantage of the existence of a privileged in-plane direction $\hat{z}$, which becomes the quantization axis of S_z when $\alpha = \beta$. When $\alpha < 0$, this system of coordinates is rotated by $\pi/2$, such that when $\alpha + \beta = 0$, the spin quantization occurs along the new $\hat{z}$ axis.

The single-particle Hamiltonian of an electron of momentum $\mathbf{p} = (p\cos\varphi, 0, p\sin\varphi)$, spin $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, and effective mass m^* is written as

$$H = \frac{p^2}{2m^*} - (\alpha + \beta)p_x\sigma_z + (\alpha - \beta)p_z\sigma_x. \tag{24}$$

The eigenvalues of the Hamiltonian are

$$\epsilon_{\pm} = \frac{p^2}{2m^*} \pm p\Delta, \tag{25}$$

where

$$\Delta = \sqrt{(\alpha + \beta)^2\cos^2\varphi + (\alpha - \beta)^2\sin^2\varphi}. \tag{26}$$

The associated eigenstates are, respectively,

$$\begin{aligned}\psi_+ &= \cos\frac{\Phi}{2}|\uparrow\rangle + \sin\frac{\Phi}{2}|\downarrow\rangle,\\ \psi_- &= -\sin\frac{\Phi}{2}|\uparrow\rangle + \cos\frac{\Phi}{2}|\downarrow\rangle,\end{aligned} \tag{27}$$

where

$$\tan\Phi = -\frac{(\alpha - \beta)}{(\alpha + \beta)}\tan\varphi. \tag{28}$$

The Fermi energy of the system is reached in each subband at maximum values of the momenta given by

$$p_{F\pm} = \sqrt{2m^*\epsilon_F + (m^*\Delta)^2} \mp m^*\Delta \tag{29}$$

if $\epsilon_F > 0$, the standard case in a 2D electron system.

The Fermi energy of the system is established by the number of particles since

$$\begin{aligned}n &= \sum_{\xi=\pm}\sum_{\mathbf{p}}\theta(p - p_\xi) = \frac{1}{(2\pi\hbar)^2}\sum_{\xi=\pm}\int_0^{2\pi}d\varphi\int_0^{p_{F\xi}}p\,dp\\ &= \frac{m^*\epsilon_F}{\pi\hbar^2} + \frac{(m^*)^2}{\pi\hbar^2}(\alpha^2 + \beta^2),\end{aligned} \tag{30}$$

where $\theta(p_F - p)$ is the Heaviside distribution in the momentum space. Consequently,

$$\epsilon_F = \frac{n\pi\hbar^2}{m^*} - m^*(\alpha^2 + \beta^2). \quad (31)$$

In a typical GaAs quantum well with particle density $n = 7 \times 10^{15}$ m^{-2} and $\beta = 4.77 \times 10^2$ m/s [9], the condition $\epsilon_F > 0$ is satisfied up to $\alpha_{\max} = 2.5 \times 10^5$ m/s, a limit much larger than one of the highest achieved values, $\alpha = 1.6 \times 10^4$ m/s (or equivalently $\hbar\alpha = 0.1$ eV Å) [16]. The variation of α is possible on account of its dependence on the potential applied across the well, while β is a characteristic of the actual structure since it is roughly proportional to the square inverse width of the quantum well multiplied by the bulk Dresselhaus constant [9].

The symmetrized spin-velocity operator is given by $\hat{\tilde{v}}_i^j = (\frac{\partial H}{\partial p_i}\sigma_j + \sigma_j\frac{\partial H}{\partial p_i})/2$, where the lower index i corresponds to the direction of propagation, while the upper index j indicates the polarization direction. Its matrix elements are evaluated immediately using Eq. (27),

$$\tilde{v}_x^x = \langle\pm|\frac{v_x\sigma_x + \sigma_x v_x}{2}|\pm\rangle = \pm\frac{p_x}{m^*}\sin\Phi, \quad (32a)$$

$$\tilde{v}_x^z = \langle\pm|\frac{v_x\sigma_z + \sigma_x v_x}{2}|\pm\rangle = \pm\frac{p_x}{m^*}\cos\Phi - (\alpha+\beta), \quad (32b)$$

$$\tilde{v}_z^x = \langle\pm|\frac{v_z\sigma_x + \sigma_x v_z}{2}|\pm\rangle = \pm\frac{p_z}{m^*}\sin\Phi + (\alpha-\beta), \quad (32c)$$

$$\tilde{v}_z^z = \langle\pm|\frac{v_z\sigma_z + \sigma_z v_z}{2}|\pm\rangle = \pm\frac{p_z}{m^*}\cos\Phi. \quad (32d)$$

The spin currents are obtained by summing all the spin velocities multiplied by $\delta f_{\mathbf{p}}^{(2)}$ for all values of the momentum in both minibands,

$$\delta j_x^x = \frac{\hbar}{2}\sum_{\xi=\pm}\sum_{\mathbf{p}}\xi\frac{p_x}{m^*}\sin\Phi\,\delta f_{\mathbf{p}}^{(2)}, \quad (33a)$$

$$\delta j_x^z = \frac{\hbar}{2}\sum_{\xi=\pm}\sum_{\mathbf{p}}\left[\xi\frac{p_x}{m^*}\cos\Phi - (\alpha+\beta)\right]\delta f_{\mathbf{p}}^{(2)}, \quad (33b)$$

$$\delta j_z^x = \frac{\hbar}{2}\sum_{\xi=\pm}\sum_{\mathbf{p}}\left[\xi\frac{p_z}{m^*}\sin\Phi + (\alpha-\beta)\right]\delta f_{\mathbf{p}}^{(2)}, \quad (33c)$$

$$\delta j_z^z = \frac{\hbar}{2}\sum_{\xi=\pm}\sum_{\mathbf{p}}\xi\frac{p_z}{m^*}\cos\Phi\,\delta f_{\mathbf{p}}^{(2)}. \quad (33d)$$

B. Electric-field-driven spin currents

In the presence of an electric field $\mathbf{E}$, the second-order distribution function is, from Eq. (22),

$$\delta f_{\mathbf{p}}^{(2)} = \frac{1}{2k_BT}(e\tau\mathbf{E}\cdot\mathbf{v}_{\mathbf{p}})^2\tanh\frac{\epsilon_{\mathbf{p}} - \epsilon_F}{2k_BT}\left(-\frac{\partial f_{\mathbf{p}}^0}{\partial\epsilon_{\mathbf{p}}}\right). \quad (34)$$

For an electric field aligned with the system axes, the spin currents are polarized perpendicular to the direction of propagation. In this case, the general computational algorithm of a spin current $j_\mu^{\bar{\mu}}$ driven by an electric field E_ν using $\delta f_{\mathbf{p}}^{(2)}$ is, from Eqs. (33) and (34),

$$\begin{aligned}\delta j_\mu^{\bar{\mu}} &= \frac{(e\tau E_\nu)^2}{16k_BT\pi^2\hbar}\sum_{\xi=\pm}\int_0^{2\pi}d\varphi\int_0^\infty d\epsilon_\xi\left[p\frac{dp}{d\epsilon_\xi}\tilde{v}_{\xi,\mu}^{\bar{\mu}}(v_{\xi,\nu})^2\right.\\&\quad\left.\times\tanh\frac{\epsilon_\xi - \epsilon_F}{2k_BT}\right]\left(-\frac{\partial f_\xi^0}{\partial\epsilon_\xi}\right)\\&= \frac{(e\tau E_\nu)^2 k_BT}{96\hbar}\sum_{\xi=\pm}\int_0^{2\pi}d\varphi\frac{d^2}{d\epsilon_\xi^2}\left[p\frac{dp}{d\epsilon_\xi}\tilde{v}_{\xi,\mu}^{\bar{\mu}}(v_{\xi,\nu})^2\right.\\&\quad\left.\times\tanh\frac{\epsilon_\xi - \epsilon_F}{2k_BT}\right]_{\epsilon_\xi=\epsilon_F}\\&= \frac{(e\tau E_\nu)^2}{96\hbar}\sum_{\xi=\pm}\int_0^{2\pi}d\varphi\frac{d}{d\epsilon_\xi}\left[p\frac{dp}{d\epsilon_\xi}\tilde{v}_{\xi,\mu}^{\bar{\mu}}(v_{\xi,\nu})^2\right]_{\epsilon_\xi=\epsilon_F},\end{aligned} \quad (35)$$

where in deriving the last two lines we used the Sommerfeld algorithm to evaluate the integrals over the energy.

Thus we obtain

$$\begin{aligned}\delta j_x^z &= \pm(\alpha+\beta)(\alpha-\beta)^2\frac{(e\tau E_{x(z)})^2}{48\hbar}\int_0^{2\pi}d\varphi\,\frac{\sin^2 2\varphi}{\Delta^2}\\&= \pm\pi(\alpha+\beta)(\alpha-\beta)^2\frac{(e\tau E_{x(z)})^2}{48\hbar\max(\alpha^2,\beta^2)}.\end{aligned} \quad (36)$$

Similarly,

$$\delta j_z^x = \pm\pi(\alpha-\beta)(\alpha+\beta)^2\frac{(e\tau E_{x(z)})^2}{48\hbar\max(\alpha^2,\beta^2)}. \quad (37)$$

The polarization of these currents is positive if driven by E_x and negative if driven by E_z.

When $\alpha \gg \beta$, both currents have the same amplitude,

$$|\delta j_\mu^{\bar{\mu}}| = \alpha\pi(e\tau E_\nu)^2/48\hbar, \quad (38)$$

a value that represents only about 60% of previous estimates for the same system parameters [13]. The currents cancel when $\alpha = \beta$, a result of the paramagnetic nature of the electron system that is spin-polarized along the $\hat{z}$ axis by the combined spin-orbit interaction, which behaves like a *de facto* magnetic field of magnitude proportional with $\alpha + \beta$ [17].

When the electric field has components along both $\hat{x}$ and $\hat{z}$ directions, E_x and E_z, respectively, the second-order distribution function symmetry permits the existence of spin currents whose polarization is along the direction of propagation. We use the general algorithm in Eq. (35) to compute δj_z^z and j_x^x. We obtain

$$\begin{aligned}\delta j_z^z &= \frac{\pi(\alpha+\beta)e^2\tau^2E_xE_z}{12\hbar}\left[1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2,\beta^2)}\right],\\\delta j_x^x &= -\frac{\pi(\alpha-\beta)e^2\tau^2E_xE_z}{12\hbar}\left[1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2,\beta^2)}\right].\end{aligned} \quad (39)$$

When $\beta = 0$, the currents are

$$\delta j_z^z = -\delta j_x^x = \frac{\alpha(e\tau)^2E_xE_z}{24\hbar}, \quad (40)$$

twice as large as that obtained when the field acts along a single axis. When $\alpha = \beta$, the currents cancel.

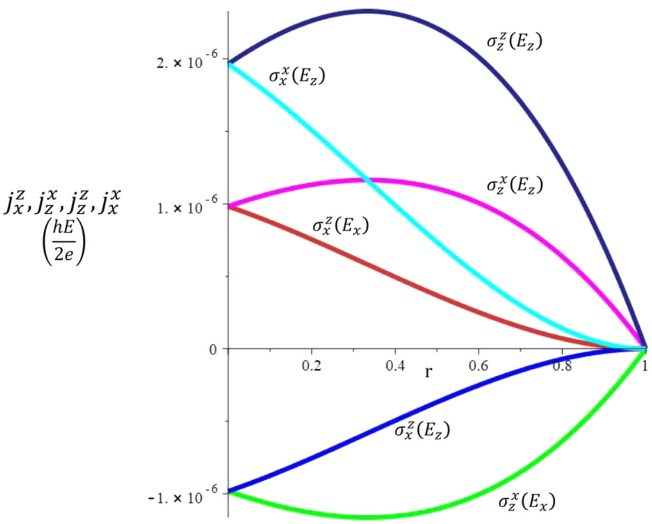

FIG. 1. The spin currents expressed in units of $\hbar E/2e$ are plotted against the ratio α/β for an intensity of the applied electric field of 10^4 V/m. The linear Dresselhaus coefficient β is 477 m/s.

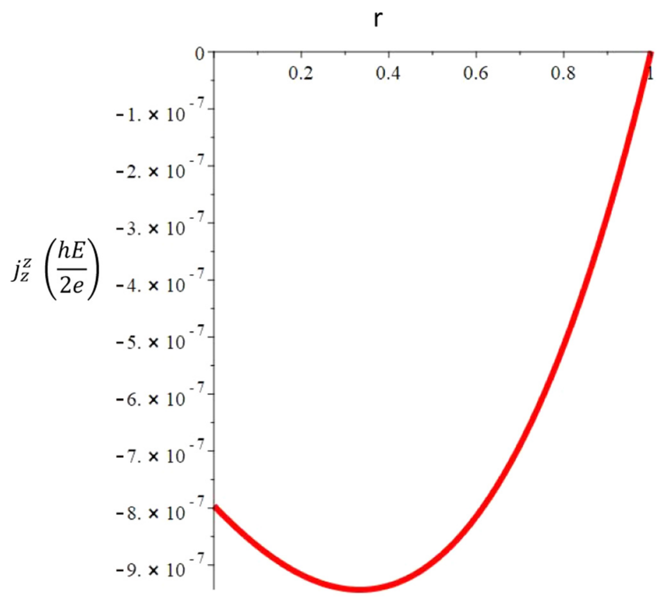

FIG. 2. The spin currents expressed in units of $\hbar E/2e$ are plotted against the ratio α/β for an applied temperature gradient $\nabla T/T$ of 10^4 m^{-1}. The linear Dresselhaus coefficient β is 477 m/s.

We illustrate our results in the case of a GaAs quantum well with electron density $n = 7 \times 10^{15}$ m^{-2}, $\beta = 4.77 \times 10^2$ m/s, and $\tau = 2.6 \times 10^{-12}$ s [9]. The currents are plotted in units of $E\hbar/2e$, since the remaining quantity has dimensions of an electric conductivity, measured in Ω^{-1}. Of course, the resulting spin-conductivity coefficient is a linear function of the electric field, so it scales proportionally with it. In Fig. 1 we plot the currents as a function of the α/β ratio for an electric field of 10^4 V/m. When $\alpha = 1.6 \times 10^4$ m/s and $\beta = 4.77 \times 10^2$ m/s, the nonlinear spin-conductivity in Eq. (37) is $3.33 \times 10^{-9}E$ Ω^{-1}. For an electric field of 10^5 V/m, it becomes 3.33×10^{-4} Ω^{-1}.

In the limit $\alpha \gg \beta$, the ratio of a nonlinear spin conductivity σ_s^2 to the usual charge conductivity $\sigma_c^{(1)} = ne^2/m^*$ can be written as, with input from Eq. (30),

$$\frac{\sigma_s^{(2)}}{\sigma_c^{(1)}} = \eta \frac{e\tau E\alpha}{\epsilon_F + m^*\alpha^2/2}, \tag{41}$$

where η is a numerical coefficient equal to $\pi^2/48$ for spin currents polarized perpendicular to the direction of propagation and to $\pi^2/24$ for those polarized along the direction of propagation. For the same system characteristics as above and for a field of 1×10^5 V/m, the ratios of the two conductivities are 2.7×10^{-2} and 5.4×10^{-2}, respectively.

C. Thermoelectric spin currents

If the temperature gradient and the electric field are applied along perpendicular directions, the angular symmetry of the second-order distribution function allows the existence of quadratic spin currents whose polarization is parallel to the direction of propagation.

In a geometry with the electric field parallel to the $\hat{x}$ axis and the temperature gradient parallel to $\hat{z}$, $\delta f_{\mathbf{p}}^{(2)}$ is given by

$$\delta f_{\mathbf{p}}^{(2)} = (eE_x\tau)(\tau\nabla_z T/T)\left[1 - \frac{1}{k_BT}(\epsilon_{\mathbf{p}} - \epsilon_F)\tanh\frac{\epsilon_{\mathbf{p}} - \epsilon_F}{2k_BT}\right] \times \left(-\frac{\partial f_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}}\right). \tag{42}$$

In this case, the only spin currents that can be driven are j_z^z and j_x^x from Eqs. (33d) and (33a). Using the same general algorithm as in Eq. (35), we obtain

$$\delta j_z^z = -\left(\frac{\pi}{12} - \frac{1}{2\pi}\right)\frac{\epsilon_F(\alpha+\beta)(e\tau E_x)(\tau\nabla_z T/T)}{\hbar} \times \left\{1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2,\beta^2)}\left[1 - \frac{m^*(\alpha^2-\beta^2)^2}{2\epsilon_F}\right]\right\},$$
$$\delta j_x^x = \left(\frac{\pi}{12} - \frac{1}{2\pi}\right)\frac{\epsilon_F(\alpha-\beta)(e\tau E_x)(\tau\nabla_z T/T)}{\hbar} \times \left\{1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2,\beta^2)}\left[1 - \frac{m^*(\alpha^2-\beta^2)^2}{2\epsilon_F}\right]\right\}. \tag{43}$$

In Fig. 2 we plot the $\hat{\mathbf{z}}$-direction spin-current that can be driven by an electric field and temperature gradient applied along perpendicular directions for the same system parameters as before. In the limit of $\alpha = \beta$, the current cancels.

For $\alpha = 1.6 \times 10^4$ m/s and $\beta = 4.77 \times 10^2$ m/s, the spin-conductivity for the thermoelectric effect is $-2.85 \times 10^{-9}\nabla T/T\,\Omega^{-1}$. The second type of thermoelectric spin currents are those driven by the quadratic temperature gradient.

From Eq. (21),

$$\delta f_{\mathbf{p}}^{(2)} = \frac{1}{2k_B T}(\epsilon_{\mathbf{p}} - \epsilon_F)^2 \tanh\frac{\epsilon_{\mathbf{p}} - \epsilon_F}{2kBT}\left(-\frac{\partial f_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}}\right) - (\epsilon_{\mathbf{p}} - \epsilon_F)\left(\tau \mathbf{v}_{\mathbf{p}} \cdot \frac{\nabla T}{T}\right)^2\left(-\frac{\partial f_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}}\right). \quad (44)$$

As before, the evaluation of current integral kernels has to proceed in the Sommerfeld algorithm. Since $\frac{\partial^2 f_{\mathbf{p}}^0}{\partial \epsilon_{\mathbf{p}}} \sim (\epsilon_{\mathbf{p}} - \epsilon_F)$, there is no contribution from the first term in (44).

Expressions for the spin-currents driven by temperature gradients applied along the system axes are derived following the general algorithm described in Eq. (35),

$$\delta j_x^z = \mp\pi \frac{(\alpha+\beta)(\alpha-\beta)^2(k_B\tau\nabla_{x(z)}T)^2}{12\hbar \max(\alpha^2, \beta^2)},$$
$$\delta j_z^x = \mp\pi \frac{(\alpha-\beta)(\alpha+\beta)^2(k_B\tau\nabla_{x(z)}T)^2}{12\hbar \max(\alpha^2, \beta^2)}, \quad (45)$$

where the spin polarization is negative when the currents are driven by temperature gradients applied along the $\hat{\mathbf{x}}$ direction and positive when the temperature gradients are along the $\hat{\mathbf{z}}$ direction.

An an in-plane temperature gradient with ∇T_x and ∇T_z components can drive spin-currents polarized along the direction of propagation,

$$\delta j_z^z = -\frac{\pi(\alpha+\beta)e^2\tau^2\nabla T_x \nabla T_z}{3\hbar}\left[1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2, \beta^2)}\right],$$
$$\delta j_x^x = \frac{\pi(\alpha-\beta)e^2\tau^2\nabla T_x \nabla T_z}{3\hbar}\left[1 - \frac{\alpha^2+\beta^2}{2\max(\alpha^2, \beta^2)}\right]. \quad (46)$$

IV. CONCLUSION

In a quadratic expansion of the Fermi distribution function written for a local energy configuration, we obtain a second-order correction to the distribution function that is proportional to the square values of the perturbative fields. The range of validity of this approximation is set equal to the distance between two electron collisions, which is proportional to τ, the relaxation time, such that the first-order correction to the function satisfies the Boltzmann transport equation. When applied to spin transport in a quantum well with competing Rashba-Dresselhaus linear interactions, our formalism generates analytic expressions for the nonlinear spin currents driven by electric fields and/or temperature gradients. The magnitude of the spin currents generated by an electric field is found to be approximately 0.6 of previous predictions. All currents cancel in the $\alpha = \beta$ limit.

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