

Spin currents, spin-transfer torque, and spin-Hall effects in relativistic quantum mechanics

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It is shown that a useful relativistic generalization of the conventional spin density $\vec{s}(\vec{r}, t)$ for the case of moving electrons is the expectation value $(\vec{T}(\vec{r}, t), \mathcal{T}_4(\vec{r}, t))$ of the four-component Bargmann-Wigner polarization operator $T_\mu = (\vec{T}, T_4)$ [Proc. Natl. Acad. Sci. U.S.A. **34**, 211 (1948)] with respect to the four components of the wave function. An exact equation of motion for this quantity is derived using the one-particle Dirac equation, and the relativistic analogs of the nonrelativistic concepts of spin currents and spin-transfer torques are identified. Using this theoretical framework, in the classical limit the Bargmann-Michel-Telegdi equation [Phys. Rev. Lett. **2**, 435 (1959)] for a relativistic wave packet crossing a nonmagnetic/ferromagnetic interface is derived, to lowest order in the spin-orbit coupling it is shown that a contribution to the polarization current occurs with spin-Hall symmetry, and the spin-transfer torque for the simple “perfect spin filter” model is calculated and discussed.

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Central to the emerging technology of spin-based electronics, often referred to as spintronics, is the observation that electron transport can be influenced not only by coupling to the charge but also by coupling to the spin of the current carrying electrons.¹ A striking example of charge current being effected by the magnetic state of the conductor is the giant magnetoresistance phenomenon. Evidently, the complementary effects of charge currents inducing changes in the magnetization of the conductors are also of interest. An example of these is the current-induced switching first predicted by Slonczewski² and independently by Berger.³ As is now well established, it is due to the spin-transfer torque that a spin-polarized current can exert on the magnetization of the structure through which it flows.⁴ However, the details of how such torques come about have not been, as yet, fully explored. In particular, all discussions of the problem are currently based on nonrelativistic quantum mechanics and hence neglect the spin-orbit coupling. The purpose of this Brief Report is to present a fully relativistic theory of spin currents and the above spin-transfer torque in order to provide a conceptual framework in which the spin and orbital degrees of freedoms can be treated on equal footing.

Another topic, to which such developments are relevant, is the spin-Hall effect intensively studied in semiconductor spintronics.^{5,6} It involves a spin current flowing perpendicularly to a charge current in a sample of finite width. Interestingly, it implies spin accumulation at the edges and the possibility of spin injection into an adjacent sample without the presence of magnetic or exchange fields. Here, spin-orbit coupling is the central issue and a source of difficulty is the lack of a well-defined spin current in a spin-orbit coupled system.⁶ It is hoped that the polarization current introduced in this Brief Report will clarify this matter considerably.

A moving electron carries with it a spin and this moving spin amounts to a spin current. Classically, it is given by the tensor product, $\vec{J}_{cl} = \vec{s}_{cl} \otimes \vec{v}$, of the velocity vector \vec{v} and a classical spin vector \vec{s}_{cl} . Quantum mechanically, for an electron described by a two-component wave function

$$\phi = \begin{pmatrix} \phi_\uparrow \\ \phi_\downarrow \end{pmatrix},$$

with spin components ϕ_\uparrow and ϕ_\downarrow , it is given by the tensor density

$$\vec{J}_s = \phi^\dagger (\vec{\sigma} \otimes \vec{J}) \phi, \quad (1)$$

where $\vec{J} = i\hbar(\vec{\nabla} - \vec{\nabla})/(2m_e)$, and the wave functions and therefore also the spin current \vec{J}_s are evaluated at the space time point (\vec{r}, t) . The physical significance of \vec{J}_s becomes apparent if we study the time evolution of the spin density defined by $\vec{s} = \phi^\dagger \vec{\sigma} \phi$. From the time-dependent Schrödinger equation which includes a Zeeman term of the form $-\mu_B \vec{\sigma} \cdot \vec{B}$, we find

$$\frac{d\vec{s}}{dt} + \nabla \cdot \vec{J}_s = \frac{e}{m_e} \vec{s} \times \vec{B}. \quad (2)$$

Clearly, $\nabla \cdot \vec{J}_s$ may be regarded as a torque which, in addition to the more familiar microscopic Landau-Lifshitz torque $\vec{s} \times \vec{B}$, causes the spin density \vec{s} at the point \vec{r} to evolve in time. As explained, at length, in the insightful review of Stiles and Miltat this spin-transfer torque depends linearly on the charge current and plays a central role in current-induced switching.⁴

Note that for $\vec{B}=0$, Eq. (2) is a continuity equation for the spin density \vec{s} and as such it follows via the Noether theorem from the fact that \vec{s} is a conserved quantity. The difficulty of generalizing the continuity equation to spin-orbit coupled systems, such as described by the Dirac equation or by various model Hamiltonians, e.g., such as those used in semiconductor spintronics,^{6,7} arises from the circumstance that in these cases the spin operator no longer commutes with the Hamiltonian and hence the conventional spin density is not conserved as the time evolves. In what follows, this dilemma is resolved by the choice of a convenient, covariant description of the spin polarization, as an alternative to that afforded by the usual spin operators in nonrelativistic quantum me-

chanics. In the following, for the sake of simplicity only the case of noninteracting positive energy Dirac electrons will be considered.

For electrons described by the Dirac equation in the standard representation, it is common to refer to

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & \mathbf{0} \\ \mathbf{0} & \vec{\sigma} \end{pmatrix} \quad (3)$$

as the 4×4 Pauli spin operator. However, it corresponds to the spin of an electron only in its rest frame and hence its use is not convenient in the case of many moving electrons. Moreover, as mentioned above, it does not commute even with the field-free Dirac Hamiltonian $\mathcal{H}_D = c\vec{\alpha} \cdot \vec{p} + \beta m_e c^2$ and hence the corresponding density is not that of a conserved quantity. A more suitable approach for describing the spin polarization of moving electrons is to use the four-component polarization operator $T_\mu \equiv (\vec{T}, T_4)$ introduced by Bargmann and Wigner.⁸ The salient features of this approach and its relations to other, alternatives, are fully discussed in a comprehensive review article by Fradkin and Good.⁹ Here, they will be merely referred to as the need arises.

For the case of one electron, in the presence of an electromagnetic field described by the vector potential $\vec{A} = \vec{A}(\vec{r}, t)$ and a scalar potential $V = V(\vec{r}, t)$, the four-component polarization operator is defined by

$$\begin{aligned} \vec{T} &= \beta \vec{\Sigma} - i \Sigma_4 \frac{\vec{\Pi}}{m_e c}, \\ T_4 &= i \vec{\Sigma} \cdot \frac{\vec{\Pi}}{m_e c}, \end{aligned} \quad (4)$$

where the canonical momentum operator takes its usual form, $\vec{\Pi} = (\vec{p} - e\vec{A})I_4$, with I_4 being the 4×4 unit matrix, and $\vec{\Sigma}$ is the spin operator defined in Eq. (3). For future reference, note that $\vec{\Sigma}$ is part of the four-component operator $\Sigma_\mu \equiv (\vec{\Sigma}, \Sigma_4)$ whose fourth component is defined as $\Sigma_4 = -i\gamma_5$ (see, e.g., Ref. 10). It is also of interest to note that both T_μ and Σ_μ are covariant axial four-vectors.

From the point of view of our present concern, the most important property of T_μ is that it commutes with the field-free Dirac Hamiltonian. Thus, as will be shown below, the corresponding vector density satisfies a continuity equation. To see the connection between the nonrelativistic spin operator $\vec{\sigma}$ and \vec{T} , it is useful to note that the latter is related to the magnetization of an electron in its rest frame by a Lorentz boost.

To derive a relativistic analog of Eq. (2), one has to calculate the first derivative with respect to the time of the polarization densities $\vec{T} = \vec{T}(\vec{r}, t)$ and $T_4 = T_4(\vec{r}, t)$ defined by

$$\vec{T} = \psi^\dagger \vec{T} \psi \quad \text{and} \quad T_4 = \psi^\dagger T_4 \psi,$$

where $\psi^\dagger = \psi^\dagger(\vec{r}, t)$ is the adjoint (conjugate transpose) of the four-component solution $\psi = \psi(\vec{r}, t)$ of the time-dependent Dirac equation corresponding to the Hamiltonian \mathcal{H}_D

$= \mathcal{H}_D(\vec{r}, t) = c\vec{\alpha} \cdot \vec{\Pi} + \beta m_e c^2 + eV I_4$. By using the chain rule for all four components $\mu = 1, \dots, 4$ in Eq. (4),

$$\frac{d\vec{T}_\mu}{dt} = \frac{\partial \psi^\dagger}{\partial t} T_\mu \psi + \psi^\dagger \frac{\partial T_\mu}{\partial t} \psi + \psi^\dagger T_\mu \frac{\partial \psi}{\partial t},$$

and the relations

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \mathcal{H}_D \psi, \quad \frac{\partial \psi^\dagger}{\partial t} = -\frac{1}{i\hbar} \psi^\dagger \mathcal{H}_D^\dagger,$$

$$\frac{\partial \vec{T}}{\partial t} = \gamma_5 \frac{e}{m_e c} \frac{\partial \vec{A}}{\partial t}, \quad \frac{\partial T_4}{\partial t} = -\frac{ie}{m_e c} \vec{\Sigma} \cdot \frac{\partial \vec{A}}{\partial t},$$

after some lengthy but straightforward algebra, one arrives at

$$\frac{d\vec{T}}{dt} + \nabla \cdot \vec{\mathcal{J}} = \frac{e}{m_e} \vec{S} \times \vec{B} - \frac{ie}{m_e c} \vec{E} S_4 \quad (5)$$

and

$$\frac{dT_4}{dt} + \nabla \cdot (\vec{\mathcal{J}}_4 - \vec{\mathcal{J}}_4'') = \frac{ie}{m_e c} \vec{S} \cdot \vec{E}, \quad (6)$$

where $\vec{B} = \vec{B}(\vec{r}, t)$ is the magnetic induction vector and $\vec{E} = \vec{E}(\vec{r}, t)$ the electric field intensity. In Eqs. (5) and (6), the four-component density $S_\mu \equiv (\vec{S}, S_4)$ is given by

$$\vec{S} = \psi^\dagger \vec{\Sigma} \psi, \quad S_4 = \psi^\dagger \Sigma_4 \psi,$$

and the polarization-current density tensors are defined as

$$\begin{aligned} \vec{\mathcal{J}}_{ij} &= c \psi^\dagger (\alpha_j T_i) \psi \quad (i, j = x, y, z), \\ \vec{\mathcal{J}}_4' &= c \psi^\dagger (T_4 \vec{\alpha}) \psi, \quad \vec{\mathcal{J}}_4'' = \psi^\dagger \left(2 \frac{\vec{\Pi}}{m_e} \times \vec{\alpha} \right) \psi \end{aligned} \quad (7)$$

such that

$$\nabla \cdot \vec{\mathcal{J}}_i = \sum_j \partial_j \vec{\mathcal{J}}_{ij}.$$

Although the above relations bear some resemblance to Eq. (2), the problem of generalizing it to relativistic quantum mechanics is not yet completed because Eqs. (5) and (6) are not a closed set of equations for the polarization density in terms of corresponding currents. To proceed further, one must derive the equation of motion for the four-component auxiliary density S_μ . Following the same route as in the case of $T_\mu \equiv (\vec{T}, T_4)$, one straightforwardly finds that

$$\frac{d\vec{S}}{dt} - ic \nabla S_4 = \frac{m_e c}{\hbar} \vec{\mathcal{J}}_4'' + i \nabla \times \vec{\mathcal{J}} \quad (8)$$

and

$$i \frac{dS_4}{dt} - c \nabla \cdot \vec{S} = i \frac{m_e c}{\hbar} \mathcal{J}'', \quad (9)$$

with $\vec{\mathcal{J}} = c \psi^\dagger \vec{\alpha} \psi$ being the relativistic probability current density and $\mathcal{J}'' = \psi^\dagger (2c\beta\gamma_5) \psi$. Remarkably, some of the same

currents which appear in the equations for \mathcal{T}_μ determine \mathcal{S}_μ and hence for a given set of currents in Eq. (7), Eqs. (5), (6), (8), and (9) can be solved for \mathcal{T}_μ and \mathcal{S}_μ .

The relations in Eqs. (5)–(9) are the central result of this Brief Report. Namely, the comparison of Eqs. (2) and (5), without electromagnetic fields, uniquely identifies the polarization-current density as $\vec{\mathcal{J}}$ and its divergence as the relativistic generalization of the conventional spin-current density and spin-transfer torque, respectively. Indeed, in the case of a vanishing electromagnetic field, Eq. (5) reduces to a continuity equation for the polarization density in the same manner as Eq. (2) is a continuity equation for the magnetization density.

To shed light on the physical content of these results, they will now be examined in two separate limits. First the classical, $\hbar \rightarrow 0$, then the nonrelativistic, $c^{-2} \rightarrow 0$, limit will be studied.

The aim of the classical limit is to find a dynamical description of the polarization of an electron whose orbital motion is classically given by the position vector $\vec{r}_{\text{cl}}(t)$ as prescribed by a relativistic classical mechanical equation of motion. In terms of the above theory, such a four-vector polarization $\tau_\mu = (\vec{\tau}, \tau_4)$ is given by

$$\vec{\tau} \equiv \vec{\tau}(t) = \int_{\Omega} d^3r \vec{\mathcal{T}}(\vec{r}, t), \quad \tau_4 \equiv \tau_4(t) = \int_{\Omega} d^3r \mathcal{T}_4(\vec{r}, t),$$

where \mathcal{T}_μ is to be calculated with respect to $\psi(\vec{r}, t)$, which describes a wave packet within a volume Ω centered at the position vector $\vec{r}_{\text{cl}}(t)$ and moving with a velocity \vec{v}_{cl} . For a linear size of the wave packet larger than the Compton wavelength \hbar/mc but very much smaller than the scale on which the external electromagnetic field varies, it follows from Eqs. (5)–(9) by using the arguments of Ref. 9 that

$$\begin{aligned} \bar{\gamma} \frac{d\vec{\tau}}{dt} + \bar{\gamma} \int_{\Omega} d^3r \nabla \cdot \vec{\mathcal{J}}(\vec{r}, t) \Big|_{\text{cl}} &= \frac{e}{m_e c} \vec{\tau} \times \vec{B}(\vec{r}_{\text{cl}}, t) \\ &\quad - i \frac{e}{m_e c} \tau_4 \vec{E}(\vec{r}_{\text{cl}}, t), \end{aligned} \quad (10)$$

where $\bar{\gamma}$ is the Lorentz factor $(1 - v^2/c^2)^{-1/2}$ and on the left-hand side the classical limit has to be taken after the volume integration. Reassuringly, Eq. (10) is exactly that of Bargmann *et al.*,¹¹ namely, the relativistic generalization of the Landau-Lifshitz equation,¹² with an extra term on the left-hand side. Consequently, by comparing Eq. (10) with Eq. (2), one readily identifies this feature as the source of spin-transfer in relativistic quantum mechanics and confirms that $\vec{\mathcal{J}}$ in Eq. (5) is indeed the fully relativistic generalization of the nonrelativistic of spin current \vec{J}_s .

Next, in what follows we examine the lowest order corrections to the nonrelativistic theory. Working to the order $1/c$, after considerable algebra we find that the equations for $\vec{\mathcal{T}}$ and $\vec{\mathcal{S}}$ satisfy one and the same equation of motion, and the polarization current is given by

$$\begin{aligned} \vec{\mathcal{J}}^{(1)} &= \phi^+ (\vec{\sigma} \otimes \vec{J}) \phi - (\phi^+ \vec{\sigma} \phi) \otimes \frac{e\vec{A}}{m_e} \\ &\quad + \frac{\hbar}{2m_e} \phi^+ \{ \vec{\sigma} \otimes [(\vec{\nabla} + \vec{\nabla}') \times \vec{\sigma}] \} \phi. \end{aligned} \quad (11)$$

Evidently, the first two terms in Eq. (11) are the generalization of the conventional \vec{J}_s in Eq. (1) to the case of a nonvanishing vector potential. The third term $\delta\vec{\mathcal{J}}^{(1)}$ is a consequence of the internal contribution to the probability current density due to the moving dipole moment $\delta\vec{J}_{\text{int}} = \hbar \nabla \times (\phi^+ \vec{\sigma} \phi) / (2m_e)$,¹² and its form readily follows from the ansatz $\delta\vec{\mathcal{J}}^{(1)} = \phi^+ (\vec{\sigma} \otimes \delta\vec{J}_{\text{int}}) \phi$.¹³ Moreover, just as $\delta\vec{J}_{\text{int}}$ does not contribute to the divergence in the continuity equation for the probability density, $\nabla \cdot \delta\vec{\mathcal{J}}^{(1)}$ is identically zero and gives rise to no torque.

To the order of $1/c^2$, there are many more contributions. These will be discussed in a separate publication. Here, only the term $\delta\vec{\mathcal{J}}_{\text{SOC}}^{(2)}$, which is clearly to be associated with the spin-orbit coupling, is highlighted:

$$\begin{aligned} \delta\vec{\mathcal{J}}_{\text{SOC}}^{(2)} &= \frac{ie\hbar}{2m_e^2 c^2} \vec{E} \cdot (\vec{\phi}^+ \vec{\sigma} \vec{\phi}) \mathbf{I}_3 \\ &\quad + \frac{e\hbar}{2m_e^2 c^2} \begin{pmatrix} 0 & +E_z & -E_y \\ -E_z & 0 & +E_x \\ +E_y & -E_x & 0 \end{pmatrix} (\vec{\phi}^+ \vec{\phi}), \end{aligned} \quad (12)$$

where $\vec{\phi}$ is ϕ renormalized as in Ref. 12.

Remarkably, the off-diagonal terms have the form required by the spin-Hall effect.⁶ It means that for an electric field, for example, and presumably a charge current, along the z axis, a spin polarization along the x axis implies a polarization current in the y direction, $j_y^x = \sigma_{\text{SH}} E_z$. Interestingly, this term is the only contribution obtained if one uses, in a simple minded derivation, the anomalous velocity,¹⁴ $\vec{v}_a = -e\hbar(\vec{\sigma} \times \vec{E}) / (4m_e^2 c^2)$, and the nonrelativistic definition of the spin-current density, $\vec{\phi}^+ [\vec{\sigma} \otimes \vec{v} + (\vec{v} \otimes \vec{\sigma})^T] \vec{\phi}$.^{6,13} Thus, the first term in Eq. (12) is a nontrivial consequence of our more general, fully relativistic treatment of the polarization. Clearly, it implies that for a charge current along the electric field, there will be a helicity-dependent contribution to the spin current.

While the above reference to the spin-Hall effect cannot be taken as an explanation for the observed spin-Hall currents due to the smallness of the vacuum coupling constant $\lambda_{\text{SOC}} = e\hbar / (2m_e^2 c^2)$ (see Ref. 6), the presence of a relevant term in Eq. (12) suggests that an intrinsic spin-Hall effect is a generic feature of spin-orbit coupled systems and therefore of the relativistic quantum mechanics.

Finally, we illustrate the use of the full theory by solving the relativistic analog of the ‘‘perfect spin filter’’ problem of Waintal *et al.*¹⁵ To proceed we consider a Dirac wave,

$$\psi_{\text{in}}(z, t) = \begin{pmatrix} u(z, t) \\ 0 \\ v(z, t) \\ 0 \end{pmatrix},$$

where u and v are the solutions of $(\varepsilon - mc^2)u = cp_z v$ and $(\varepsilon + mc^2)v = cp_z u$ incident along the z axis onto an interface in the xy plane between a nonferromagnet and a ferromagnet magnetized in the x direction. This state is an eigenstate of Σ_z with eigenvalue $+1$ and can be decomposed as follows:

$$\begin{pmatrix} u \\ 0 \\ v \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left[\frac{1}{\sqrt{2}} \begin{pmatrix} u \\ -u \\ v \\ v \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} u \\ u \\ v \\ -v \end{pmatrix} \right],$$

where the states on the right-hand side are solutions of the Dirac equation. Simultaneously, they are eigenstates of the polarization operator $T_z = \beta \Sigma_z$ corresponding to ± 1 , respectively. Thus, as in the nonrelativistic case, we assume that the component with polarization parallel to the target (whose orientation is \vec{e}_x) is transmitted, and the one with polarization along $-\vec{e}_x$ is reflected, namely,

$$\psi_{\text{ref}}(z, t) = \frac{1}{\sqrt{2}} \begin{pmatrix} u^*(z, t) \\ -u^*(z, t) \\ v^*(z, t) \\ v^*(z, t) \end{pmatrix}$$

and

$$\psi_{\text{tr}}(z, t) = \frac{1}{\sqrt{2}} \begin{pmatrix} u(z, t) \\ u(z, t) \\ v(z, t) \\ -v(z, t) \end{pmatrix}.$$

Using these wave functions to calculate the polarization-current tensor given in Eq. (7), by carrying out the surface

integral over the pillbox of volume Ω including the interface, we find that the torque is nonvanishing in the z direction, and is given by

$$\int_{\Omega} d^3r \nabla \cdot \vec{\mathcal{J}} = \frac{\langle p_z \rangle}{m_e} = v_z \left(1 - \frac{v_z^2}{c^2} \right)^{-1/2},$$

where $\langle p_z \rangle$ is the expectation value of $-i\hbar \partial_z$ with respect to $\psi_{\text{in}}(z, t)$ and v_z is the usual relativistic velocity of the electron constituting the current. This expression is clearly a relativistic generalization of the nonrelativistic result as given in Ref. 15 and implies that in the ultrarelativistic limit the torque tends to infinity.

In conclusion, it should be stressed that the above discussion was confined to a one-electron theory based on a one-electron Dirac equation. Nevertheless, the results establish the line of reasoning a relativistic generalization of the corresponding many-particle theory has to take. In particular, it will lead to a relativistic version of the semiclassical transport theory for the current-induced switching dynamics⁴ or for that of the spin-Hall effect.¹⁶ It will also facilitate the corresponding generalization of the time-dependent density functional theory of Capelle *et al.*,¹⁷ and will readily provide a framework for first-principles calculation using fully relativistic methods such as the screened relativistic Korringa-Kohn-Rostoker (RKKR) method.¹⁸ Interestingly, it will also enter the relativistic Fermi liquid theory of Baym and Chin.¹⁹

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