Description of spin transport and precession in spin-orbit coupling systems and general equation of continuity

Hua-Tong Yang\textsuperscript{1} and Chengshi Liu\textsuperscript{2}
\textsuperscript{1}School of Physics, Peking University, Beijing 100871, China
\textsuperscript{2}Department of Mathematics, Daqing Petroleum Institute, Daqing 163318, China

By generalizing the usual current density to a matrix with respect to spin variables, a general equation of continuity satisfied by the density matrix and current density matrix has been derived. This equation holds in arbitrary spin-orbit coupling systems as long as its Hamiltonian can be expressed in terms of a power series in momentum. Thereby, the expressions of the current density matrix and a torque density matrix are obtained. The current density matrix completely describes both the usual current and spin current as well: while the torque density matrix describes the spin precession caused by a total effective magnetic field, which may include a realistic and an effective one due to the spin-orbit coupling. In contrast to the conventional definition of spin current, this expression contains an additional term if the Hamiltonian includes nonlinear spin-orbit couplings. Moreover, if the degree of the full Hamiltonian $\geq 3$, then the particle current must also be modified in order to satisfy the local conservation law of number.

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I. INTRODUCTION

Recently, the spin transport, precession, and accumulation generated by spin-orbit coupling and the resulting intrinsic spin-Hall effect\textsuperscript{1,2} have attracted considerable interest by physicists\textsuperscript{3,4,5,6,7,8,9,10,11,12,13} because it may provide a promising method to manipulate the electronic spin without application of magnetic field\textsuperscript{14,15,16,17} in spintronics.\textsuperscript{18,19} However, some conceptual ambiguities still remain in how to properly describe the spin transport and precession in spin-orbit coupling systems. In order to describe these phenomena, a conventional spin current operator is intuitively defined as $\hat{J}_j^i = (1/2)\{\hat{v}_i, \hat{s}_j\}$, with $\hat{v}_i = \partial H/\partial p$, a velocity operator and $\hat{s}_j$ a spin component (actually, as will be pointed out in Sec. IV, this expression should also contain a factor of density operator $\delta(x-x)$ in order to have the dimension of a current density). However, it is still very questionable whether this quantity is meaningfully observable. This problem has caused a lot of confusion and debates in recent literature\textsuperscript{20,21,22,23,24,25} and has even become an obstacle to the further progress of this filed. From the experimental point of view, the most interesting observable is the spin density,\textsuperscript{15,16,17} which can be given by $\text{tr}(\hat{s}_j \hat{\rho})$, with

$$\hat{\rho} = \begin{bmatrix} \rho_{\uparrow\uparrow} & \rho_{\uparrow\downarrow} \\ \rho_{\downarrow\uparrow} & \rho_{\downarrow\downarrow} \end{bmatrix}$$

the density matrix; i.e., the density matrix $\hat{\rho}$ can completely describe the number density as well as its spin polarization. Theoretically, a fundamental equation describing a transport phenomenon of any additive conserved quantity, say $Q$, is the equation of continuity $\partial \rho_Q/\partial t + \nabla \cdot \hat{J}_Q = 0$, which connects the change of its density $\rho_Q$ to a corresponding current $\hat{J}_Q$: if this additive quantity is not conserved, we must introduce a source (or drain) term $S_Q$ in this equation such that $\partial \rho_Q/\partial t + \nabla \cdot \hat{J}_Q = S_Q$. As a classical picture of motion, the spin transport in spin-orbit coupling systems is very similar to the latter case, since the spin is also an additive and local quantity (the locality means that the spin commutes with the position); i.e., the spin density can be defined as a function of position. Therefore, a straightforward approach to introduce the spin current is to establish a continuitylike equation satisfied by the density matrix $\hat{\rho}$. This equation should be a general counterpart of the usual continuity equation of number $\partial \rho/\partial t + \nabla \cdot \hat{J} = 0$, and can be called a general continuity equation. We expect that a corresponding current density matrix $\hat{J}$ can be naturally obtained from it. However, as the spin is not conserved, so the time rate of change of $\hat{\rho}$ must contain two distinct parts, i.e., $\partial \hat{\rho}/\partial t = -\nabla \cdot \hat{J} + \hat{T}$. The first part is a divergence $-\nabla \cdot \hat{J}$, which can be ascribed to a current density matrix $\hat{J}$; while the second one, denoted by $\hat{T}$, does not possess this character and can be called a torque density matrix. If we integrate both sides of this equation over a volume $\Omega$, then we have $\partial \rho/\partial t \int_{\Omega} \hat{\rho} dV = -\oint_{\partial \Omega} \hat{\rho} \nabla \cdot \hat{J} + \int_{\Omega} \hat{T} dV$. The surface integral $\oint_{\partial \Omega} \hat{\rho} \nabla \cdot \hat{J} dS$ can be interpreted as a current flowing through the boundary surface $\partial \Omega$, while the volume integral $\int_{\Omega} \hat{T} dV$ represents the precession rate of the spin polarization within the volume $\Omega$. As will be demonstrated in Sec. II, this division can be uniquely determined by the equation of motion $\partial \hat{\rho}/\partial t = [\hat{H}(\hat{p}, \hat{x}), \hat{\rho}] = \mathcal{L}[\hat{\rho}(\hat{x}, \hat{x}'; t)]$ and the condition that $\hat{T}$ can no longer be expressed as a divergence, where $\mathcal{L}[\hat{\rho}] = (\nabla, \nabla') \hat{\rho}$ is a functional operator acting on $\hat{\rho}$ and $\nabla = \nabla_{\hat{x}}$ and $\nabla' = \nabla_{\hat{x}'}$ are the differentiation operators with respect to $\hat{x}$ and $\hat{x}'$, respectively. The
essence of this problem is to cast the $\mathcal{L}[\hat{\rho}]$ into the form

$$
\mathcal{L}(\nabla, \nabla')[\hat{\rho}] = (\nabla + \nabla') \cdot \hat{\mathcal{J}}[\hat{\rho}] + T(\frac{1}{2}(\nabla - \nabla'))[\hat{\rho},],
$$

where $\hat{\mathcal{J}}(\nabla, \nabla')[\hat{\rho}]$ and $T(\frac{1}{2}(\nabla - \nabla'))[\hat{\rho}]$ are also functional operators. It will be proven that $\hat{\mathcal{J}}$ and $T$ can be uniquely determined by the equation of motion as long as $\mathcal{L}$ can be written as a power series in $\nabla$ and $\nabla'$. So, if we define

$$
\hat{J}(x) = -\lim_{x' \to x} \hat{\mathcal{J}}(\nabla, \nabla')[\hat{\rho}(x, x')],
$$

$$
T(x) = \lim_{x' \to x} T(\frac{1}{2}(\nabla - \nabla'))[\hat{\rho}(x, x')],
$$

then the continuity-like equation can be obtained. It is important to note that if we transform the $\hat{\rho}(x, x')$ to the Wigner function $\hat{\rho}(\mathbf{p}, \mathbf{R})$, where $\mathbf{R} = \frac{1}{2}(x + x')$ and $\mathbf{p}$ is the canonical momentum corresponding to $x - x'$, then the expression for $T$ has the form $T(\mathbf{R}) = \int d^3\mathbf{p} T(i\mathbf{p})[\hat{\rho}(\mathbf{p}, \mathbf{R})]$; it no longer contains the spatial derivative $\nabla$ and, therefore, cannot be written as a divergence.

From this general continuity equation, we can deduce that the $\text{tr}\hat{\mathcal{J}}$ and $\text{tr}(\hat{s}\hat{\mathcal{J}})$ represent the current density of particle $\mathbf{J}$ and the current density of spin $\mathbf{J}^s$, respectively, just as the $\text{tr}\hat{\rho}$ and $\text{tr}(\hat{s}\hat{\rho})$ represent the number density $\rho$ and spin density $\rho_s(x)$, respectively, i.e., the matrix $\hat{J}$ can provide a complete description of the particle transport as well as the spin transport. In order to confirm that this physical interpretation is self-consistent, we must prove that

1. $\text{tr}\hat{T} \equiv 0$, which is a necessary and sufficient condition for the local conservation of number and
2. $\mathbf{J}$ and $\hat{T}$ must be gauge invariant in order to ensure that they can be interpreted as physically observable. In this paper, a general equation of continuity satisfied by $\hat{\rho}$, $\hat{J}$ and $\hat{T}$ is derived, which holds in arbitrary spin-orbit coupling systems as long as its Hamiltonian can be written as a polynomial in momentum. Consequently, the expressions of the $\mathbf{J}$ and $\mathbf{T}$ are presented. These expressions are gauge invariant and independent of the magnitude of spin and the system dimension and satisfy $\text{tr}\hat{T} \equiv 0$. In contrast to the conventional definition, this formulism contains the following corrections: First, if the spin-orbit coupling Hamiltonian includes second- or higher order power of momentum, e.g., in the Luttinger model, the two-dimensional (2D) cubic Rashba model or the Dresselhaus spin-orbit coupling, then we should add a new additional term to the expression for $\mathbf{J}$, which is purely originated from the nonlinear spin-orbit coupling and contributes only to the spin current. Second, if the degree of the full Hamiltonian $\text{deg}\hat{H}(\mathbf{p}) \geq 3$, e.g., in the cubic Rashba model or Dresselhaus spin-orbit term, then the particle current density $\mathbf{J}$ as well as the spin current density are also different from the conventional definition; otherwise, it will violate the local conservation law of number. Moreover, this equation of continuity also holds in the presence of arbitrary electromagnetic field and Coulomb interaction or nonmagnetic impurity scattering. Consequently, from this continuity-like equation we can also deduce some exact identities which are very similar to the Ward-Takahashi identity, although the spin is not a conserved quantity.

This paper is organized as follows. In Sec. II the general equation of continuity in a spin-orbit coupling system without Coulomb interaction and impurity scattering is derived. Then, we will prove that this equation also holds in the presence of the Coulomb interaction and nonmagnetic impurities in Sec. III. Section IV is devoted to a detailed discussion and comparison of these expressions with the conventional intuitive definition. A short summary of the conclusions will be given in Sec. V.

II. GENERAL EQUATION OF CONTINUITY

Firstly, we consider a general spin-orbit coupling system without any two-body interaction or impurity scattering, but may subject to an external electromagnetic field described by $(\phi, \mathbf{A})$; the case in the presence of the Coulomb interaction or impurity scattering will be discussed in Sec. III. The corresponding one-body Hamiltonian has the form

$$
\hat{H} = \frac{1}{2m} \left( \mathbf{P} - \frac{e}{c} \mathbf{A} \right)^2 + e\phi + \hat{h}_{so} = \hat{h}_0 + e\phi + \hat{h}_{so},
$$

where $\hat{h}_0 \equiv (1/2m)(\mathbf{P} - \frac{e}{c} \mathbf{A})^2$ is the kinetic energy and $\hat{h}_{so}$ is a general spin-orbit coupling Hamiltonian and we suppose it can be expanded as a power series

$$
\hat{h}_{so} = \hat{H}^{(0)} + \hat{H}_i^{(1)} \hat{p}_i + \hat{H}_{ij}^{(2)} \hat{p}_i \hat{p}_j + \hat{H}_{ijk}^{(3)} \hat{p}_i \hat{p}_j \hat{p}_k + \cdots.
$$
Here and hereafter, a summation over repeated suffix is implied, where \( \hat{p}_i \equiv -i\hbar \partial_i - (e/c) A_i \equiv -i\hbar \partial_i \ (i = x, y, z) \), \( \partial_i \) are the covariant derivatives, and \( \hat{H}^{(n)}_{i_1 \ldots i_n} \ (n = 0, 1, 2, \ldots) \) are the components acting on spin variable (or \( 2 \times 2 \) matrixes if the spin is \( 1/2 \)); meanwhile, \( \hat{H}^{(0)} \) is a scalar representing Zeeman energy due to magnetic field, \( \hat{H}^{(1)}_i \) are the components of a vector, \( \hat{H}^{(n)}_{i_1 \ldots i_n} \) are the components of a tensor of rank \( n \) and are supposed to be symmetric under the permutations of its suffixes \( i_1, i_2, \ldots, i_n \). Furthermore, we assume that all \( \hat{H}^{(n)}_{i_1 \ldots i_n} \) are independent of position except \( \hat{H}^{(0)} \). The corresponding many-body Hamiltonian is \( \hat{H} = \int \psi^\dagger_\alpha(1) \hat{H}_{\sigma\sigma'} \psi_{\sigma'}(1) \), where \( \sigma \) and \( \sigma' \) are spin variables.

In order to derive the general equation of continuity, we consider the equation of motion of Green’s function for this approach is apparently gauge invariant. The density matrix \( \hat{\rho} \) can be given by \( \rho_{\alpha\beta}(xt) = C \langle \exp \{-i\hat{\mathcal{F}}[\psi_\alpha(xt)\psi_{\beta}^\dagger(xt^+)]\} = -i\hbar G_{\alpha\beta}(xt, xt^+) \), where \( \hat{\mathcal{F}} \) is the time-ordering operator and \( t^+ = t + 0^+ \). From the equation of motion we have

\[
\left( i\hbar \frac{\partial}{\partial t} - e\phi(1) \right) \hat{G}(1, 1') - \frac{\hbar}{\hbar} \hat{h}_{so} \hat{G}(1, 1') = 0,
\]

where \( \hat{G} \) denotes the matrix \( G_{\alpha\beta} \), and \( (1) \equiv (xt), (1') \equiv (xt') \). By taking the limit as \( 1' \to 1^+ \), the first term becomes

\[
\lim_{1' \to 1^+} \left[ i\hbar \frac{\partial}{\partial t} - e\phi(1) + i\hbar \frac{\partial}{\partial t'} + e\phi(1') \right] \hat{G}(1, 1') = -\frac{\partial \hat{\rho}(xt)}{\partial t}.
\]

The commutator \([\hat{h}_0, \hat{G}]\) in the second term of Eq. (3) can be written as

\[
[\hat{h}_0, \hat{G}] = \left[ \mathcal{P} - \frac{e}{c} \mathcal{A}, \frac{1}{2m} \left\{ \mathcal{P} - \frac{e}{c} \mathcal{A}, \hat{G}(1, 1') \right\} \right],
\]

where \( (\mathcal{P} - (e/c) \mathcal{A}) \hat{G}(1, 1') \equiv [-i\hbar \nabla - (e/c) \mathcal{A}(1)] \hat{G}(1, 1'), \hat{G}(1, 1')(\mathcal{P} - (e/c) \mathcal{A}) \equiv [i\hbar \nabla' - (e/c) \mathcal{A}(1')] \hat{G}(1, 1'), [\hat{\mathcal{X}}, \hat{\mathcal{Y}}] \equiv \sum_{i} \left[ \hat{X}_i, \hat{Y}_i \right], \) and \( \{\hat{\mathcal{X}}, \hat{\mathcal{Z}}\} \equiv \sum_{i} \{\hat{X}_i, \hat{Z}_i \} \). Because

\[
\lim_{1' \to 1^+} \left\{ \mathcal{P} - \frac{e}{c} \mathcal{A}, \hat{G}(1, 1') \right\} = \frac{i}{\hbar} \left\{ \mathcal{P} - \frac{e}{c} \mathcal{A}, \hat{\rho}(1, 1') \right\} \bigg|_{1' = 1},
\]

so, if we define a current density matrix

\[
\hat{J}_0(1) \equiv \frac{1}{2m} \left\{ \mathcal{P} - \frac{e}{c} \mathcal{A}, \hat{\rho}(1, 1') \right\}_1',
\]

then we have

\[
\lim_{1' \to 1^+} \left[ \hat{h}_0, \hat{G}(1, 1') \right] = \nabla \cdot \hat{J}_0(xt).
\]

Now, we consider the spin-orbit coupling term \([\hat{h}_{so}, \hat{G}(1, 1')]\). According to Eq. (2), the first term is simply

\[
\lim_{1' \to 1^+} \left[ \hat{H}^{(0)}, \hat{G} \right] = -\frac{1}{\hbar} \left[ \hat{H}^{(0)}, \hat{\rho} \right]\bigg|_{1' = 1},
\]

In order to treat the other terms of \([\hat{h}_{so}, \hat{G}(1, 1')]\), we note that \( \hat{H}^{(n)}_{i_1 \ldots i_n} \ (n \geq 1) \) commute with \( \hat{\rho} \) because they are independent of the position, and use the following operator relation: if \([\hat{A}, \hat{B}] = 0\), then \([\hat{A}\hat{B}, \hat{C}] = (1/2)\{\hat{A}, [\hat{B}, \hat{C}] + (1/2)[\hat{A}, \{\hat{B}, \hat{C}\}] \). By substituting Eq. (2) into \([\hat{h}_{so}, \hat{G}(1, 1')]\), we obtain

\[
[\hat{h}_{so}, \hat{G}] = \frac{1}{2} \sum_{n} \left( \left\{ \hat{H}^{(n)}_{i_1 \ldots i_n}, \hat{p}_{i_1} \ldots \hat{p}_{i_n}, \hat{G} \right\} + \left[ \hat{H}^{(n)}_{i_1 \ldots i_n}, \left\{ \hat{p}_{i_1} \ldots \hat{p}_{i_n}, \hat{G} \right\} \right] \right),
\]

where

\[
\left\{ \hat{p}_{i_1} \ldots \hat{p}_{i_n}, \hat{G} \right\} \equiv \left( \hat{p}_{i_1} \ldots \hat{p}_{i_n} + \hat{p}_{i_1}' \ldots \hat{p}_{i_n}' \right) \hat{G}(1, 1'),
\]

\[
\left[ \hat{p}_{i_1} \ldots \hat{p}_{i_n}, \hat{G} \right\} \equiv \left[ \hat{p}_{i_1} \ldots \hat{p}_{i_n} - \hat{p}_{i_1}' \ldots \hat{p}_{i_n}' \right] \hat{G}(1, 1'),
\]
and $\hat{p}_{j'}^n \equiv i\hbar \partial_j' - (e/c)A_j'(1') \equiv i\hbar \tilde{\partial}_j'$, which commute with $\hat{p}_i$ because $\hat{p}_i$ act on $1 = (x, t)$ while $\hat{p}_{j'}$ act on $1' = (x', t')$. It is easy to verify that Eq. (7) is also a special case of identity (8). The limit of the first term on the right-hand side of Eq. (8) can be entirely written as a divergence form. For $n = 1$, we have

$$\lim_{\gamma \to 1} \frac{1}{2} \left\langle H_i^{(1)}(1), \left[ \hat{p}_i, \tilde{G} \right] \right\rangle = \nabla \cdot \frac{1}{2} \left\{ H_i^{(1)}, \left[ \hat{p}_i(1), 1' \right] \right\} \left|_{1' = 1} \right.,$$

where $H^{(1)} = (\tilde{H}_y^{(1)}, \tilde{H}_z^{(1)})$. For $n \equiv m + 1 \geq 2$, we define an auxiliary operator

$$\hat{D}_{i_1 \cdots i_m}^{(m)}(\hat{p}_i, \hat{p}'_i) \equiv \hat{p}_{i_1} \cdots \hat{p}_{i_m} + \hat{p}_{i_1} \cdots \hat{p}_{i_{m-1}} \hat{p}'_{i_m} + \cdots + \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m-1}} \hat{p}_{i_m} = \sum_{l=0}^{m} \hat{p}_{i_1} \cdots \hat{p}_{i_{m-l}} \hat{p}'_{i_{m-l+1}} \cdots \hat{p}'_{i_m}. \tag{12}$$

Owing to the symmetry of $\hat{G}_{i_1 \cdots i_m}$ and commutability between $\hat{p}_i$ and $\hat{p}_{j'}$, we have

$$\frac{1}{2} \left\{ \hat{H}_{i_1 i_2 \cdots i_{m+1}}^{(m+1)}, \left[ \hat{p}_{i_1} \hat{p}_{i_2} \cdots \hat{p}_{i_{m+1}}, \hat{G}(1, 1') \right] \right\} = (\hat{p}_{i_1} - \hat{p}'_{i_1}) \frac{1}{2} \left\{ \hat{H}_{i_1 i_2 \cdots i_m}^{(m+1)}, \hat{D}_{i_1 \cdots i_m}^{(m)}(\hat{p}_i, \hat{p}'_i) \hat{G}(1, 1') \right\}. \tag{13}$$

So, if we define

$$(\hat{J}_{so})_i \equiv \sum_m \frac{1}{2} \left\{ \hat{H}_{i_1 i_2 \cdots i_m}^{(m+1)}, \hat{D}_{i_1 \cdots i_m}^{(m)}(\hat{p}_i, \hat{p}'_i) \hat{G}(1, 1') \right\} \left|_{1' = 1} \right.,$$

where we also introduce a $\hat{\mathcal{D}}^{(0)} \equiv 1$ in order to include the term of Eq. (11) in this unified formula, then we have

$$\lim_{\gamma \to 1} \sum_n \frac{1}{2} \left\{ \hat{H}_{i_1 \cdots i_n}^{(n)}, \left[ \hat{p}_{i_1} \cdots \hat{p}_{i_n}, \hat{G}(1, 1') \right] \right\} = \partial_i (\hat{J}_{so})_i = \nabla \cdot \hat{J}_{so}. \tag{15}$$

The limit of the second term $\frac{1}{2} \left\{ \hat{H}_{i_1 \cdots i_n}^{(n)}, \left\{ \hat{p}_{i_1} \cdots \hat{p}_{i_n}, \hat{G} \right\} \right\}$ on the right-hand side of Eq. (8) cannot be entirely written as a divergence. However, we can prove that it can be written as a divergence and a remaining term, while the remaining term no longer contains spatial derivatives $\nabla \mathbf{R}$ if it is represented by the Wigner distribution function. In order to prove this conclusion, we take first the case when $n = 1$, it evidently cannot be written as a divergence as $1' \to 1^+$, because $\left\{ \hat{p}_i, \hat{G} \right\} = -i\hbar (\partial_i - \partial_{i'}) \hat{G}(1, 1')$ and only the limit of $(\partial_i + \partial_{i'})$ can be written as a divergence. Then, we take $n \equiv m + 1 \geq 2$ and prove that the limits of

$$\hat{H}_{i_1 i_2 \cdots i_n}^{(n)} \left\{ \hat{p}_{i_1} \hat{p}_{i_2} \cdots \hat{p}_{i_n}, \hat{G} \right\} - 2\hat{\mathcal{H}}_{i_1 i_2 \cdots i_n}^{(n)} \frac{1}{2} \frac{\hat{p}_{i_1} + \hat{p}'_{i_1}}{2} \cdots \frac{\hat{p}_{i_n} + \hat{p}'_{i_n}}{2} \hat{G},$$

and

$$\left\{ \hat{p}_{i_1} \hat{p}_{i_2} \cdots \hat{p}_{i_n}, \hat{G} \right\} \hat{H}_{i_1 i_2 \cdots i_n}^{(n)} - 2\hat{\mathcal{H}}_{i_1 i_2 \cdots i_n}^{(n)} \frac{1}{2} \frac{\hat{p}_{i_1} + \hat{p}'_{i_1}}{2} \cdots \frac{\hat{p}_{i_n} + \hat{p}'_{i_n}}{2} \hat{G} \hat{H}_{i_1 i_2 \cdots i_n}^{(n)}$$

can be written as a divergence form. To this end, we again introduce the following auxiliary operators:

$$\hat{R}_{i_1 \cdots i_n}^{(n)}(\hat{p}_i, \hat{p}'_i) \equiv \frac{\hat{p}_{i_1} + \hat{p}'_{i_1}}{2} \cdots \frac{\hat{p}_{i_n} + \hat{p}'_{i_n}}{2},$$

and define another term of the current density matrix $\hat{J}_{so}$ as

$$(\hat{J}_{so})_i \equiv \sum_{m \geq 1} \frac{1}{4} \left\{ \hat{H}_{i_1 i_2 \cdots i_m}^{(m+1)}, \hat{\mathcal{G}}_{i_1 \cdots i_m}^{(m)}(\hat{p}_i, \hat{p}'_i) \hat{G}(1, 1') \right\} \left|_{1' = 1} \right.,$$

and a torque density matrix as

$$\hat{T}[\hat{\mathcal{R}}] \equiv \sum_n \frac{1}{4i\hbar} \left\{ \hat{H}_{i_1 i_2 \cdots i_n}^{(n)}, \hat{R}_{i_1 i_2 \cdots i_n}^{(n)}(\hat{p}_i, \hat{p}'_i) \hat{G}(1, 1') \right\} \left|_{1' = 1} \right..$$
It is easy to verify that the terms of \( n = 0, 1 \) can also be incorporated into the right-hand side of definition (19) if we define \( \tilde{R}^{(0)} \equiv 1 \). Then, we can prove that (see the Appendix A)

\[
\lim_{y \to 1, \nu} \sum_{n} \frac{1}{2} \left[ \hat{H}^{(n)}_{1i\cdots i_n} \left\{ \hat{p}_i, \hat{\rho}_{i_2} \cdots \hat{\rho}_{i_n}, \hat{\gamma} \right\} \right] = \nabla \cdot \hat{J}_s - \hat{T}[\hat{\rho}], \tag{20}
\]

where \( \hat{J}'_s \) is a new term of the current density matrix, which is originated from the nonlinear spin-orbit coupling, because it will vanish if \( \hat{H}^{(n)}_{1i\cdots i_n} \) are independent of spin (i.e., it is only a c-number rather than a spin matrix). More importantly, we should note that the \( \hat{T}[\hat{\rho}] \) cannot be rewritten as a divergence because it is given by a polynomial of \( \hat{\rho} - \hat{\gamma} \). This property will be more evident if we transform the \( \hat{\rho}(1, 1') \) to a gauge-invariant Wigner distribution function \( \tilde{\rho} \) by

\[
\tilde{\rho}_{\alpha\beta}(\tilde{p}, \tilde{\varepsilon}; \mathbf{R}, t) = \int d^3 \tilde{r} d\tau e^{i[\tilde{\varepsilon} + \tilde{\varepsilon}(\mathbf{R} t)] - \tilde{p}\tilde{A}(\mathbf{R} t) \cdot \tilde{r}} \langle \psi^{\dagger}_\beta(R - \frac{\mathbf{p}}{2} t - \frac{\mathbf{r}}{2}, \mathbf{p} + \frac{\mathbf{r}}{2} t + \frac{\mathbf{r}}{2}) | \psi_\alpha(R + \frac{\mathbf{p}}{2} t + \frac{\mathbf{r}}{2}) \rangle,
\]

in which the macroscopic variables \( \mathbf{R} = (x + x')/2 \) and microscopic variables \( \mathbf{r} = x - x' \) have been used, and then we have

\[
\left[ \hat{H}^{(n)}_{1i\cdots i_n}, \hat{R}^{(n)}_{1i\cdots i_n} \right]_{\nu = 1} = \int \frac{d^3 \tilde{p} d\tilde{v}}{(2\pi)^3} \left[ \hat{H}^{(n)}_{1i\cdots i_n} \hat{p}_{i_2} \cdots \hat{p}_{i_n}, \tilde{\rho}(\tilde{p}, \tilde{\varepsilon}; \mathbf{R}, t) \right]. \tag{21}
\]

It does not involve the macroscopic spatial derivative \( \nabla_{\mathbf{R}} \), and therefore can not be written as a divergence \( \nabla_{\mathbf{R}} \cdot \mathbf{J} \). Comparing this expression with Eq. (7), it is obvious that the \( \hat{H}^{(n)}_{1i\cdots i_n} \hat{p}_{i_2} \cdots \hat{p}_{i_n} \) plays a role which is very similar to Zeeman energy \( \hat{H}^{(0)} \). The only difference is that the former depends on momentum, because it is originated from the spin-orbit coupling, while the latter depends on position. So, the \( \hat{H}^{(n)}_{1i\cdots i_n} \hat{p}_{i_2} \cdots \hat{p}_{i_n} \) can be regarded as the energy contributed by an effective magnetic field depending on momentum. Take the limit as \( 1' \to 1^+ \) and substituting Eq. (7), (9), (15) and (20) into Eq. (3), we finally obtain the following generalized equation of continuity:

\[
\frac{\partial \tilde{\rho}}{\partial t} + \nabla \cdot \left( \mathbf{J}_0 + \mathbf{J}_s + \mathbf{J}'_s \right) = \hat{T}[\tilde{\rho}]. \tag{22}
\]

Evidently, the form of this equation is independent of the system dimension or the magnitude of spin. The only differences are the number of components of the current density and the dimension of the matrices, if the system dimension or the spin magnitude are different.

From the definitions (5), (13), (18), and (19), we can deduce that \( \hat{\mathbf{J}} \) and \( \hat{T} \) are gauge invariant because all the derivatives in their definitions are covariant. Moreover, from the definitions (18) and (19), we get \( \text{tr} \hat{J}_s' \equiv 0 \) and \( \text{tr} (\hat{T}[\hat{\rho}]) \equiv 0 \), owing to their commutator form. The identity \( \text{tr} [\hat{T}[\hat{\rho}]] \equiv 0 \) ensures the local conservation law of number (or charge), while \( \text{tr} \hat{J}_s' \equiv 0 \) means that the \( \mathbf{J}'_s \) does not contribute to the particle or charge current, but it may contribute to the spin current. Because \( \text{tr} \hat{\rho}(\mathbf{x} t) \) is the number density \( \rho(\mathbf{x} t) \), so, \( \text{tr} \mathbf{J}(\mathbf{x} t) = \text{tr} (\mathbf{J}_0 + \mathbf{J}_s) \) is the current density of the particle \( \mathbf{J}(\mathbf{x} t) \), while the charge current is \( \mathbf{J}_c(\mathbf{x} t) = e \mathbf{J}(\mathbf{x} t) \), here the identity \( \text{tr} \hat{J}_s' \equiv 0 \) has been used. By letting \( \mathbf{J}_0 = \text{tr} \hat{\mathbf{J}}_0 \) and \( \mathbf{J}_s = \text{tr} \hat{\mathbf{J}}_s \) and taking the trace over spin of both sides of the Eq. (22), we obtain the conservation law

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{J}_0 + \mathbf{J}_s) = 0. \tag{23}
\]

Similarly, because

\[
\rho_s(\mathbf{x} t) \equiv \text{tr} [\hat{\rho}(\mathbf{x} t) \hat{s}] = \text{tr} [\hat{s} \hat{\rho}(\mathbf{x} t)] = \frac{1}{2} \text{tr} \{ \hat{\rho}, \hat{s} \} \tag{24}
\]

is the expectation value of the spin density, therefore, it is natural to define the spin current density as

\[
\mathbf{J}^s(\mathbf{x} t) \equiv \text{tr} \left[ \hat{\mathbf{J}}(\mathbf{x} t) \hat{s} \right] = \text{tr} \left[ \hat{s} \hat{\mathbf{J}}(\mathbf{x} t) \right] = \frac{1}{2} \text{tr} \{ \hat{\mathbf{J}}, \hat{s} \} \tag{25}
\]

and the spin torque density as

\[
T^s(\mathbf{x} t) \equiv \text{tr} \left[ \hat{T}(\mathbf{x} t) \hat{s} \right] = \text{tr} \left[ \hat{s} \hat{T}(\mathbf{x} t) \right] = \frac{1}{2} \text{tr} \{ \hat{T}, \hat{s} \}. \tag{26}
\]
From Eq. (22), we obtain the following equation of continuity satisfied by the spin density, spin current density and spin torque density:

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot J^s = T^s.
\] (27)

This equation and Eqs. (19) and (21) reveal that the matrix \( \hat{T} \) completely describes the spin precession caused by a total effective magnetic field, which may contain both the Zeeman term and the effective magnetic field originated from the spin-orbit coupling.

A potential question is that whether the torque density matrix \( \hat{T} \) can also be rewritten as a divergence by solving the equation \( \hat{T} = -\nabla \cdot \mathbf{J}_T \) although the expression for \( \hat{T} \) itself no longer explicitly contains spatial derivatives \( \nabla R \). This is not practicable, because the condition \( \hat{T} = -\nabla \cdot \mathbf{J}_T \) is not sufficient to uniquely determine the expression for \( \mathbf{J}_T \) except in one-dimensional systems, since the \( \mathbf{J}_T \) will have two or three unknown components in a 2D or three-dimensional systems, but there is only one equation, which is evidently not sufficient.\[^{35}\] The physical meaning of this conclusion is that the precession rate \( \int_{\Omega} \hat{T} dV \) in a volume \( \Omega \) cannot be determined only by the information on the boundary surface \( \partial \Omega \), i.e., it cannot be expressed by a surface integral such as a current. In contrast, the effect of the term \( \nabla \cdot \mathbf{J}_s \) can be expressed as a surface integral \( \int_{\partial \Omega} \mathbf{J}_s \cdot d\mathbf{S} \) if we consider \( (\partial / \partial t) \int_{\Omega} \hat{\rho} d^3 \mathbf{R} \). Furthermore, from definitions (17) and (15), we can find that there is a common factor \( \hat{\rho}_i - \hat{\rho}'_i = -i\hbar \partial R_i \) in the expression for \( \mathbf{J}_s \), which implies that the term \( \int_{\partial \Omega} \mathbf{J}_s \cdot d\mathbf{S} \) may still be nonvanishing when there are no no electrons inside the volume \( \Omega \), i.e., \( \hat{\rho}(\mathbf{R}) = 0 \) for all \( \mathbf{R} \in \Omega \), because the derivatives \( \partial \hat{\rho} / \partial R_i \) on the boundary may include a nonvanishing spin polarized part. So, it may give a nonvanishing \( \mathbf{J}_s \), and the \( (\partial / \partial t) \int_{\Omega} \hat{\rho} d^3 \mathbf{R} \) may also be nonvanishing; it turns out that the time evolution rate of the total spin inside the volume is nonvanishing even when there are no electrons. Therefore, the \( \int_{\partial \Omega} \mathbf{J}_s \cdot d\mathbf{S} \) can only be interpreted as another kind of current flowing from the outside of the volume \( \Omega \), since in this case there are no spins (or electrons) inside the volume; so, it is impossible to be explained as the spin precession inside the volume.

III. THE INFLUENCE OF THE COULOMB INTERACTION AND THE SCATTERING BY NONMAGNETIC IMPURITIES

Now, we consider the influence of the Coulomb interaction, which can be written as

\[
\mathbf{H}_c = \frac{1}{2} \int d1d1'\psi_{\sigma(1)}^\dagger(1')\psi_{\sigma(1)}(1')v(1 - 1')\psi_{\sigma(1)}^\dagger(1')\psi_{\sigma(1)},
\] (28)

where \( v(1 - 1') \) is independent of spin. So, the total Hamiltonian is \( \mathbf{H} + \mathbf{H}_c \), and Eq. (4) becomes\[^{36}\] \( \hat{G}_{0}^{-1}\hat{G} - \hat{G}_{0}\hat{G}^{-1} \) becomes

\[
[\hat{G}_{0}^{-1}\hat{G} - \hat{G}_{0}\hat{G}^{-1}]_{\alpha,\beta}(1,1') = -i\hbar \int [v(1 - 2) - v(1' - 2)]G_{\alpha\gamma,\gamma\beta}(12^{-},1'2^{+}),
\] (29)

where \( [\hat{G}_{0}^{-1}\hat{G}](1,1') = i\hbar(\partial / \partial t)\hat{G}(1,1') - \hat{h}(1)\hat{G}(1,1') \) and \( [\hat{G}\hat{G}_{0}^{-1}](1,1') = -i\hbar(\partial / \partial t')\hat{G}(1,1') - \hat{G}(1,1')\hat{h}(1') \); \( G_{\alpha\gamma,\gamma\beta}(12^{-},1'2^{+}) = [1/(i\hbar)^2]([\pi|\hat{\psi}_{\alpha}(1)|\hat{\psi}_{\gamma}(2)]\psi_{\beta}(1')\psi_{\beta}(1')) \) is the two-particle Green’s function, and a bar over variable (2) indicates that it is the integral variable, \( 2^{-} = (x_2, t_2 - 0^{+}) \). As \( 1' \to 1^{+} \), the left-hand side of Eq. (29) is \( \hat{T}[\hat{\rho}] - (\partial \hat{\rho} / \partial t) - \nabla \cdot \mathbf{J} \), while the right-hand side will vanish because

\[
[v(1 - 2) - v(1' - 2)]_{1' = 1} = 0.
\]

Therefore, we again obtain the Eq. (22).

We take into account the scattering of some random nonmagnetic impurities and suppose that the impurity potential has the form \( U(x; \{ \mathbf{r}_i \}) = \sum_i u(x - \mathbf{r}_i) \), with \( \mathbf{r}_i \) is the position of \( i \)th impurity and here \( U(\{ \mathbf{r}_i \}) \) is a function of the set \( \{ \mathbf{r}_i \} \). The additional term of the second-quantized Hamiltonian \( \mathbf{H}_{imp}(\{ \mathbf{r}_i \}) = \int d1U(1; \{ \mathbf{r}_i \})\psi_{\beta}(1')\psi_{\beta}(1) \) Now, the interesting quantities become some quantities averaged over these random impurity positions, e.g., \( \hat{\rho}(1) \equiv \int \cdots \int \prod_i (d^3\mathbf{r}_i / \Omega)\hat{\rho}(1; \{ \mathbf{r}_i \}) \), and \( \overline{\mathbf{J}}(1) \equiv \int \cdots \int \prod_i (d^3\mathbf{r}_i / \Omega)\overline{\mathbf{J}}(1; \{ \mathbf{r}_i \}) \), etc., where \( \Omega \) is the volume of the system. So, the Eq. (4) becomes

\[
\left[i\hbar \frac{\partial}{\partial t} - e\phi(1) + i\hbar \frac{\partial}{\partial t'} + e\phi(1') \right] \hat{G}(\{ \mathbf{r}_i \}) - \left[ \hat{h} + U(\{ \mathbf{r}_i \}), \hat{G}(\{ \mathbf{r}_i \}) \right] = 0.
\] (30)
Because $U$ is independent of spin, we have
\[
\lim_{\tau \to 1^+} |U(\{r_i\}, \hat{G}(1, 1'; \{r_i\})| = \lim_{\tau \to 1^+} |U(1, \{r_i\}) - U(1, \{r_i\})\hat{G}(1, 1'; \{r_i\})| = 0.
\]
Therefore, we get
\[
\frac{\partial \hat{\rho}(x; \{r_i\})}{\partial t} + \nabla \cdot \hat{J}(x; \{r_i\}) = \hat{T} [\hat{\rho}(\{r_i\})].
\]
(31)

By taking the ensemble average with respect to $\{r_i\}$ of both sides of this equation, we have
\[
\int \cdots \int \prod_i \frac{d^3 r_i}{\Omega} \left[ \frac{\partial \hat{\rho}(x; \{r_i\})}{\partial t} + \nabla \cdot \hat{J}(x; \{r_i\}) \right] = \int \cdots \int \prod_i \frac{d^3 r_i}{\Omega} \hat{T} [\hat{\rho}(\{r_i\})],
\]
interchange the ordering of the integrations and differentiations, we obtain
\[
\frac{\partial \hat{\rho}}{\partial t} + \nabla \cdot \hat{J} = \hat{T} [\hat{\rho}].
\]
(32)

Similarly, it is can also be proved that this equation still holds if the Coulomb interaction and the impurity scattering exist simultaneously. Furthermore, if we take the functional differentiations with respect to the external fields on both sides of this equation, we will obtain some exact identities connecting the correlation functions of the spin current, spin torque, and the usual particle current, which will be very similar to the usual Ward-Takahashi identity even though the spin is not a conserved quantity. So, if we use some approximation methods to calculate the response of the spin current or spin torque to external perturbations, then the self-consistency must be taken into account in order to preserve these exact identities, just as in the problem of the electron transport. In addition, these expressions can also be applied to the finite temperature systems, only if all averages are defined with respect to a grand canonical ensemble, in which the spin-orbit coupling terms will appear as a thermodynamic weighting factor \(\exp(-\mathbf{H}_{so}/kT)\). Because the spin-orbit coupling coefficients are often very small, so Green's functions and the related observables may appear as spin polarized only if the temperature is low enough such that $\mathbf{H}_{so}/kT$ can not be ignored. Otherwise, this weighting factor will be almost spin isotropic, so the phenomena due to the spin polarization will be unobservable.

### IV. DISCUSSIONS AND COMPARISONS

The expressions derived in Sec. II, which are expressed in terms of density matrix, can also be given by the corresponding one-body operators such that $\langle \hat{f} \rangle = \text{tr} \int d\mathbf{x} d\mathbf{x}' \hat{f}(\mathbf{x}', \mathbf{x}) \hat{\rho}(\mathbf{x}, \mathbf{x}') \equiv \text{Tr}(\hat{f} \hat{\rho})$, where $\hat{f}(\mathbf{x}', \mathbf{x}) = \langle \mathbf{x}' | \hat{f}(\hat{\mathbf{p}}, \hat{\mathbf{x}}) | \mathbf{x} \rangle$ represents a one-body operator; "Tr" denotes the trace over both the spin and coordinate variables (while the "tr" is the trace over spin). This form is more convenient to compare with the conventional definition, since the latter was usually given by a one-body operator. To this end, we need only to consider a special case $\hat{\rho}(\mathbf{x}, \mathbf{x}') = \psi(\mathbf{x})\psi^*(\mathbf{x}')$ and obtain the following relation:
\[
[\hat{p}_{i_1} \cdots \hat{p}_{i_m} \hat{p}_{j_1}' \cdots \hat{p}_{j_n}'] \hat{\rho}(\mathbf{x}, \mathbf{x}')|_{\mathbf{x}' = \mathbf{x}} = \langle \psi | \hat{p}_{j_1} \cdots \hat{p}_{j_n} \delta(\mathbf{x} - \mathbf{x}) \hat{p}_{i_1} \cdots \hat{p}_{i_m} | \psi \rangle
\]
\[
= \left[ \left( -i\hbar \delta_{j_1} \right) \cdots \left( -i\hbar \delta_{j_n} \right) \psi(\mathbf{x}) \right]^* \left[ \left( -i\hbar \delta_{i_1} \right) \cdots \left( -i\hbar \delta_{i_m} \right) \psi(\mathbf{x}) \right],
\]
(33)

where $\mathbf{x}$ is the position operator and $\mathbf{x}$ is the eigenvalue of $\hat{x}$ [note that $\delta(\mathbf{x} - \mathbf{x}) = |\mathbf{x}\rangle \langle \mathbf{x}|$ is the probability density operator]. Here, the spin suffixes are ignored for simplicity. From this relation, we have the following corresponding rule:
\[
\hat{p}_{i_1} \cdots \hat{p}_{i_m} \hat{p}_{j_1}' \cdots \hat{p}_{j_n}' \iff \hat{p}_{j_1} \cdots \hat{p}_{j_n} \delta(\mathbf{x} - \mathbf{x}) \hat{p}_{i_1} \cdots \hat{p}_{i_m}.
\]
(34)

According to this rule, we can obtain the corresponding one-body operators of $\mathbf{J}_0$, $\mathbf{j}_{0, s}$, $\mathbf{J}_{so}$, $(\mathbf{j}_{so})'$, and $\mathbf{T}$, which will be denoted by $\hat{j}_0$, $\hat{j}_0$, $\hat{j}_{so}$, $\hat{j}_{so}'$, and $\hat{T}$, respectively. From definitions $\hat{j}_0$ and $\mathbf{J}_0 = \text{tr} \mathbf{J}_0$, we have
\[
\hat{j}_0 = \frac{1}{2m} \{\hat{p}, \delta(\hat{x} - \mathbf{x})\}
\]
(35)
and its mean value \( \langle \psi | \hat{J}_0 | \psi \rangle = (i\hbar/2m) \left[ (\nabla \psi)^* \psi - \psi^* \nabla \psi \right] \). Its contribution to spin current density is

\[
\hat{j}_0^s = \frac{1}{4} \left\{ \hat{s}, \left\{ \frac{\hat{p}}{m}, \delta(\hat{x} - \hat{x}) \right\} \right\} = \frac{1}{2} \{ \hat{s}, \hat{j}_0 \}.
\]  

(36)

In order to express the one-body operators \( \hat{j}_0 \) and \( \hat{j}_0^s \), we define

\[
\hat{d}^{(m)}_{i_1 \cdots i_m}(\hat{p}, \hat{x}) \equiv \delta(\hat{x} - \hat{x}) \hat{p}_{i_1} \cdots \hat{p}_{i_m} + \hat{p}_{i_m} \delta(\hat{x} - \hat{x}) \hat{p}_{i_1} \cdots \hat{p}_{i_{m-1}} + \cdots + \hat{p}_{i_1} \cdots \hat{p}_{i_{m-2}} \delta(\hat{x} - \hat{x}).
\]  

(37)

This is the one-body operator corresponding to definition (12). According to definition (13), \( \hat{J}_{so} = \text{tr} \hat{J}_{so} \), and \( \hat{J}_{so}^s = \text{tr} (\hat{s} \hat{J}_{so}) \), we obtain that the term of particle current density \( \hat{j}_{so} \) can be given by

\[
\langle \hat{j}_{so} \rangle_i = \sum_m \frac{1}{2} \{ \hat{s}, \hat{d}^{(m+1)}_{i_1 \cdots i_m} \} \hat{d}^{(m)}_{i_1 \cdots i_m}(\hat{p}, \hat{x}),
\]  

(38)

while its corresponding spin current density can be given by

\[
\langle \hat{j}_{so}^s \rangle_i = \sum_m \frac{1}{2} \{ \hat{s}, \hat{d}^{(m+1)}_{i_1 \cdots i_m} \} \hat{d}^{(m)}_{i_1 \cdots i_m}(\hat{p}, \hat{x}) = \frac{1}{2} \{ \hat{s}, \langle \hat{j}_{so} \rangle_i \}.
\]  

(39)

Similarly, let

\[
\hat{r}^{(m)}_{i_1 i_2 \cdots i_m} = \left\{ \frac{\hat{p}_{i_1}}{2}, \left\{ \frac{\hat{p}_{i_2}}{2}, \ldots, \left\{ \frac{\hat{p}_{i_m}}{2}, \delta(\hat{x} - \hat{x}) \right\} \ldots \right\} \right\}
\]  

(40)

and

\[
\hat{c}^{(m)}_{i_1 i_2 \cdots i_m} = [\hat{p}_{i_1} \cdots \hat{p}_{i_m}, \delta(\hat{x} - \hat{x})] + [\hat{p}_{i_1} \cdots \hat{p}_{i_{m-1}}, \hat{r}^{(1)}_{i_m}] + \cdots + [\hat{p}_{i_1} \hat{r}^{(m-1)}_{i_2 \cdots i_m}].
\]  

(41)

From definitions (18), (19), (25) and (26) we have

\[
\langle \hat{j}_{so}^s \rangle_i = \sum_{m \geq 1} \frac{1}{4} \{ \hat{s}, \hat{d}^{(m+1)}_{i_1 \cdots i_m} \} \hat{c}^{(m)}_{i_1 \cdots i_m},
\]  

(42)

\[
\hat{r}^s = \sum_{n} \frac{1}{i\hbar} \left[ \hat{s}, \hat{d}^{(n)}_{i_1 i_2 \cdots i_m} \right] \hat{r}^{(n)}_{i_1 i_2 \cdots i_m}.
\]  

(43)

In order to compare these expressions with the conventional definition, we must first clarify a misleading statement in the conventional definition. In recent literature, the spin current was usually defined as \( \hat{J}^s = \frac{1}{2} \{ \hat{v}, \hat{s} \} \). However, what we are actually concerned is not the mean value of this operator \( \langle \psi | \hat{J}^s | \psi \rangle \), but the mean value of some kind of density of this operator \( \frac{1}{2} | \psi(\hat{x}) \rangle \langle \hat{x} | \hat{J}^s | \psi(\hat{x}) \rangle + \langle \hat{J}^s \psi(\hat{x}) | \psi(\hat{x}) \rangle = \langle \psi | \frac{1}{2} \{ \hat{J}^s, \delta(\hat{x} - \hat{x}) \} | \psi \rangle \). Therefore, more precisely, the quantity we actually defined is \( \frac{1}{4} \{ \{ \hat{v}, \hat{s} \}, \delta(\hat{x} - \hat{x}) \} \) rather than \( \frac{1}{2} \{ \hat{v}, \hat{s} \} \) itself and should be called a spin current density. Moreover, the spin current, by analogy with any other kind of current, should be defined as an integral \( I^s[A] = \int_A \hat{j}_0^s dA \) of the spin current density \( \hat{j}_0^s \) over a surface \( A \), which is also not the \( \frac{1}{4} \{ \hat{v}, \hat{s} \} \) itself. Now, a puzzle that confronted us is that there exist some different Hermitian combinations of the products of \( \hat{v}, \delta(\hat{x} - \hat{x}) \) and \( \hat{s} \) because they do not commute in spin-orbit coupling systems. They all have the same dimension and the same classical analogy (or classical limit), it is very difficult to determine which one should be interpreted as the proper spin current density just by this intuitive method. For example, we can also define \( \frac{1}{4} \{ \{ \hat{v}, \hat{s} \}, \delta(\hat{x} - \hat{x}) \} \) or \( \frac{1}{4} \{ \{ \hat{v}, \delta(\hat{x} - \hat{x}) \}, \hat{s} \} \) as a spin current density (only the first one and the third one are equal owing to the fact that \( \hat{s} \) and \( \hat{x} \) commute). From the classical picture of motion, the physical meaning of the second one can be interpreted as the velocity multiplied by the spin density, while third one is the particle current density multiplied by spin. Moreover, if the velocity includes higher power of momentum, i.e., it is a nonlinear function of momentum, then there will be even more probable expressions of the operator due to the noncommutative property of the density (or position) and momentum. According to the results given above, the spin current density must include two different parts in order to satisfy the generalized continuity equation. The first part is \( \hat{j}_0^s + \hat{j}_{so}^s \), it can be written as \( \frac{1}{2} \{ \hat{s}, \hat{j}_0 + \hat{j}_{so} \} \). However, the \( \hat{j}_{so} \) cannot be simply written as \( \hat{j}_0 = \frac{1}{2} \left\{ \frac{\partial \hat{h}}{\partial \hat{p}}, \delta(\hat{x} - \hat{x}) \right\} \) (only the \( \hat{j}_0 \) does) but should be written as a more complex expression given by Eq. (38). These two expressions are
equal only if the velocity operator \( \frac{\partial \hat{H}(\hat{p})}{\partial \hat{p}} \) is a linear function of \( \hat{p} \) (correspondingly, the degree of the full Hamiltonian must satisfies \( \deg \hat{H}(\hat{p}) \leq 2 \)). The second part \( \langle \hat{p}_i \rangle \) is originated from the nonlinear spin-orbit coupling terms, it appears only if \( \deg \hat{\rho}_{\text{so}}(\hat{p}) \geq 2 \) and takes the form of commutator instead of anticommutator. From the viewpoint of noncommutativity of operators, this new term is originated from the noncommutativity of the density operator \( \hat{\delta}(\hat{x} - \hat{x}) \) and the \( d\hat{s}/dt \), because the latter one also includes momentum operators in spin-orbit coupling systems. This term does not give any additional contribution to the particle current (or charge current) but may contribute an additional surface integral term if we consider the time rate of change of the total spin in a given volume.

As an example of these differences, we can consider a model with the following Dresselhaus spin-orbit coupling,\(^{27,28,29}\) in which

\[
\hat{h}_{\text{so}} = \frac{\gamma}{2} \sum_i \sigma_i \hat{p}_i (\hat{p}^2_i + 1 - \hat{p}^2_i + 2), \quad (i = x, y, z; \quad i + 3 \rightarrow i),
\]

where \( \sigma_i \) are the Pauli matrices. After symmetrization, it can be rewritten as \( \hat{h}_{\text{so}} = \hat{H}^{(3)}_{\text{xy}} \hat{p}_x \hat{p}_y \hat{p}_z \), where \( \hat{H}^{(3)}_{\text{xy}} = \hat{H}^{(3)}_{\text{yy}} = -\hat{H}^{(3)}_{\text{zz}} = -\hat{H}^{(3)}_{\text{xx}} = -\hat{H}^{(3)}_{\text{yz}} = \hat{H}^{(3)}_{\text{zy}} = \hat{H}^{(3)}_{\text{zx}} = -\hat{H}^{(3)}_{\text{yz}} = -\hat{H}^{(3)}_{\text{xy}} = \hat{H}^{(3)}_{\text{xx}} = \hat{H}^{(3)}_{\text{yy}} = \hat{H}^{(3)}_{\text{zz}}, \) and all the other \( \hat{H}^{(3)}_{i_1 \cdots i_n} = 0 \). Because the \( \hat{J}_0 \) always has the same form for arbitrary model, so, here we only give the expression for \( \hat{J}_{\text{so}}, \hat{J}_v \) and \( \hat{T} \). According to the definitions \( \hat{E}_4 \), \( \hat{E}_8 \) and \( \hat{E}_9 \), we have

\[
\langle \hat{J}_{\text{so}} \rangle_x = \frac{\gamma}{6} \left\{ \hat{\sigma}_x \left[ \hat{D}^{(2)}_{\text{yy}} - \hat{D}^{(2)}_{\text{zz}} \right] \hat{\rho} - \{ \hat{\sigma}_y, [\hat{D}^{(2)}_{\text{zy}} + \hat{D}^{(2)}_{\text{yz}}] \hat{\rho} \} + \{ \hat{\sigma}_z, [\hat{D}^{(2)}_{\text{xx}} + \hat{D}^{(2)}_{\text{xy}}] \hat{\rho} \} \right\}
= \frac{\gamma}{6} \{ \hat{\sigma}_x, \hat{p}_x \hat{p}_y + \hat{p}_y \hat{p}_z + \hat{p}_z \hat{p}_y - \hat{p}_y \hat{p}_y - \hat{p}_z \hat{p}_z - \hat{p}_z \hat{p}_z \} \hat{\rho} - \{ \hat{\sigma}_y, [\hat{p}_x \hat{p}_y + \hat{p}_y \hat{p}_x + \hat{p}_y \hat{p}_y + \hat{p}_z \hat{p}_z + \hat{p}_z \hat{p}_y + \hat{p}_y \hat{p}_z] \hat{\rho} \} + \{ \hat{\sigma}_z, [\hat{p}_x \hat{p}_x + \hat{p}_z \hat{p}_z + \hat{p}_z \hat{p}_x + \hat{p}_z \hat{p}_y + \hat{p}_y \hat{p}_z + \hat{p}_y \hat{p}_y] \hat{\rho} \} \}
\]

\[
\langle \hat{J}_v \rangle_x = \frac{\gamma}{12} \left\{ \{ \hat{\sigma}_x, [\hat{C}^{(2)}_{\text{yy}} - \hat{C}^{(2)}_{\text{zz}}] \hat{\rho} \} - \{ \hat{\sigma}_y, [\hat{C}^{(2)}_{\text{zy}} + \hat{C}^{(2)}_{\text{yz}}] \hat{\rho} \} + \{ \hat{\sigma}_z, [\hat{C}^{(2)}_{\text{xx}} + \hat{C}^{(2)}_{\text{xy}}] \hat{\rho} \} \right\}
= \frac{\gamma}{12} \{ \{ \hat{\sigma}_x, \hat{p}_y \hat{p}_y - \hat{p}_z \hat{p}_z - \hat{p}_z \hat{p}_z \} \hat{\rho} - \{ \hat{\sigma}_y, [\hat{p}_x \hat{p}_y + \hat{p}_y \hat{p}_x + \hat{p}_z \hat{p}_y + \hat{p}_y \hat{p}_z + \hat{p}_y \hat{p}_y] \hat{\rho} \} + \{ \hat{\sigma}_z, [\hat{p}_x \hat{p}_x + \hat{p}_z \hat{p}_z + \hat{p}_z \hat{p}_x + \hat{p}_z \hat{p}_y + \hat{p}_y \hat{p}_z + \hat{p}_y \hat{p}_y] \hat{\rho} \} \}
\]

The \( y \) and \( z \) components can be obtained by permutations of the suffixes according to the rule \( x \rightarrow y, y \rightarrow z, z \rightarrow x \) and \( x \rightarrow z, z \rightarrow y, y \rightarrow x \), respectively. The spin torque density is

\[
\hat{T}[\hat{\rho}] = \frac{\gamma}{2\hbar} \sum_i \left\{ \hat{\sigma}_i, \frac{1}{2} \{ \hat{p}_i + \hat{p}_i' \} \left( (\hat{p}_{i+1} + \hat{p}_{i+1}')^2 - (\hat{p}_{i+2} + \hat{p}_{i+2}')^2 \right) \right\} \}
\]

For this model, \( \hat{J}_{\text{so}} \) cannot be simply given by \( \frac{1}{2} \{ \hat{v}_{\text{so}}, \hat{\delta}(\hat{x} - \hat{x}) \} \) with \( \hat{v}_{\text{so}} = \partial \hat{h}_{\text{so}}(\hat{p})/\partial \hat{p} \), although their results correspond to the same classical analogy. Because the latter intuitive definition all terms such as \( \hat{p}_x \hat{p}_y \), \( \hat{p}_x \hat{p}_y \) etc. are replaced by \( \hat{p}_x \hat{p}_x \) (or \( \hat{p}_x \hat{p}_y \)), and \( \hat{p}_x \hat{p}_y \) (or \( \hat{p}_x \hat{p}_y \)), respectively, so it obviously violates the local equation of continuity. Moreover, the new term \( \hat{J}'_{\text{so}} \), which is purely originated from the nonlinear spin-orbit interaction and cannot be given by intuitive method, must also be taken into account in order to satisfy the continuity equation.

**V. SUMMARY**

In conclusion, by defining a current and a torque density matrix, a general equation of continuity satisfied by the matrixes of the density, current density and torque density has been derived. This equation holds in spin-orbit coupling systems as long as their Hamiltonian can be expressed in terms of a power series in momentum. Thereby, the universal expressions of the current density matrix and torque density matrix have been uniquely determined. The current density matrix can completely describe the particle (or charge) current as well as the spin current in a unified form, while the torque density matrix represents spin precession caused by a total magnetic field, including a usual and an effective one. This effective magnetic field is originated from the spin-orbit coupling and depends on momentum. In contrast to the conventional intuitive definition, it is found that if the spin-orbit coupling Hamiltonian includes nonlinear term of momentum, then the definition of the current density matrix should contain a new additional term, which is purely originated from the nonlinear spin-orbit coupling and can only contribute to the spin current. Moreover, if the degree of the full Hamiltonian \( \geq 3 \), then the conventional intuitive definition of the current density must also be modified in order to satisfy the local conservation law of number.
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APPENDIX A: DERIVATION OF EQ. (20)

Because (1) $\hat{p}_i$ is commute with $\hat{p}'_i$, and (2) $H_{i_1 \cdots i_m}^{(n)}$ is symmetric under the interchange of its suffixes, we have

$$\hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \left( \hat{p}_{i_1} \cdots \hat{p}_{i_{m+1}} - \hat{R}_{i_1 \cdots i_{m+1}}^{(m+1)} \right) \hat{G}(1, 1') = \frac{1}{2} (\hat{p}_i - \hat{p}'_i) \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{F}_{i_1 \cdots i_{m+1}}^{(m)} \hat{G}(1, 1'),$$

(A1)

$$\hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \left( \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m+1}} - \hat{R}_{i_1 \cdots i_{m+1}}^{(m+1)} \right) \hat{G}(1, 1') = -\frac{1}{2} (\hat{p}_i - \hat{p}'_i) \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{F}_{i_1 \cdots i_{m+1}}^{(m)} \hat{G}(1, 1'),$$

(A2)

where

$$\hat{F}_{i_1 \cdots i_{m}}^{(m)} = \hat{p}_{i_1} \cdots \hat{p}_{i_{m}} + \hat{p}_{i_1} \cdots \hat{p}_{i_{m-1}} \hat{R}_{i_m}^{(1)} + \cdots + \hat{R}_{i_1 \cdots i_{m}}^{(m)},$$

(A3)

$$\hat{F}_{i_1 \cdots i_{m}}^{(m)} = \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m}} + \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m-1}} \hat{R}_{i_m}^{(1)} + \cdots + \hat{R}_{i_1 \cdots i_{m}}^{(m)}.$$  

(A4)

Therefore, we get

$$\hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \left( \hat{p}_{i_1} \cdots \hat{p}_{i_{m+1}}, \hat{G} \right) - 2 \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{R}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{G} = \frac{1}{2} (\hat{p}_i - \hat{p}'_i) \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{C}_{i_1 \cdots i_{m+1}}^{(m)} \hat{G},$$

(A5)

where

$$\hat{C}_{i_1 \cdots i_{m}}^{(m)} = \hat{F}_{i_1 \cdots i_{m}}^{(m)} - \hat{F}_{i_1 \cdots i_{m}}^{(m)} = \hat{p}_{i_1} \cdots \hat{p}_{i_{m}} + \hat{p}_{i_1} \cdots \hat{p}_{i_{m-1}} \hat{R}_{i_m}^{(1)} + \cdots + \hat{R}_{i_1 \cdots i_{m}}^{(m)} - \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m}} - \hat{p}'_{i_1} \cdots \hat{p}'_{i_{m-1}} \hat{R}_{i_m}^{(1)} + \cdots + \hat{R}_{i_1 \cdots i_{m}}^{(m)}. $$

(A6)

Similarly, we have

$$\left( \hat{p}_{i_1} \cdots \hat{p}_{i_{m+1}}, \hat{G} \right) \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} - 2 \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{G} \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} = \frac{1}{2} (\hat{p}_i - \hat{p}'_i) \hat{C}_{i_1 \cdots i_{m+1}}^{(m)} \hat{G} \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)}.$$  

(A7)

Adding Eq. (A5) and (A7), we get

$$\frac{1}{2} \left[ \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \left( \hat{p}_{i_1} \cdots \hat{p}_{i_{m+1}}, \hat{G} \right) \right] = \frac{1}{4} (\hat{p}_i - \hat{p}'_i) \left[ \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{C}_{i_1 \cdots i_{m+1}}^{(m)} \hat{G} + \hat{H}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{R}_{i_1 \cdots i_{m+1}}^{(m+1)} \hat{G} \right].$$

(A8)

By taking the limit as $1' \to 1^+$, we obtain the Eq. (20).
This nonuniqueness can also be verified by considering some concrete examples. e.g., in a 2D circle of radius $R$, the vector field $\mathbf{V}(x) = f(r)(-y/r, x/r)$ defined inside this circle obviously satisfies $\nabla \cdot \mathbf{V}(x) = 0$, here $f(r)$ is arbitrary differentiable function satisfying $f(0) = f(R) = 0$, $r$ is the distance between $(x, y)$ and $(0, 0)$, so, the solution of $\nabla \cdot \mathbf{J}(x) = T$ is unique when even the boundary condition is given, it can be arbitrarily altered by $\mathbf{J} + \mathbf{V}$. For 3D system, the solution of the equation $\nabla \cdot \mathbf{J}(x) = T$ can be altered by $\mathbf{J} + \nabla \times \mathbf{F}$, where $\mathbf{F}$ is an arbitrary vector field. 

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