

## Probability- and spin-current operators for effective Hamiltonians

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(Received 13 July 2011; revised manuscript received 7 February 2012; published 14 June 2012)

We present a systematic construction of the probability- and spin-current operators, based on a momentum power expansion of effective Hamiltonians. These operators play an essential role in transport problems related to semiconductor heterostructures, in particular when spin-orbit interaction is taken into account. The result, valid whatever the momentum power and including the linear (Bychkov-Rashba) term as well as the cubic (Dresselhaus or D'yakonov-Perel) term, is of special importance for spintronics.

DOI: [10.1103/PhysRevB.85.235313](https://doi.org/10.1103/PhysRevB.85.235313)

PACS number(s): 72.25.Dc, 71.70.Ej, 73.40.Gk

### I. INTRODUCTION

The probability current is a fundamental concept in quantum mechanics, which connects the wavelike description of a quasiparticle to the notion of the transport current. When we consider a general Schrödinger problem with the Hamiltonian

$$\hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m} + \mathcal{U}(\mathbf{r}), \quad (1.1)$$

where the real potential  $\mathcal{U}(\mathbf{r})$  is periodic in a crystalline solid and  $m$  is the free-electron mass, we are led to the usual definition of the free-electron probability current:<sup>1</sup>

$$\mathbf{J}^f = \text{Re} \left[ \psi^* \frac{\hat{\mathbf{p}}}{m} \psi \right] = \frac{\hbar}{m} \text{Im} [\psi^* \nabla \psi]. \quad (1.2)$$

When the spin-orbit interaction (SOI) is taken into account, the Hamiltonian becomes

$$\hat{H} = \hat{H}_0 + \hat{H}_{SO} \quad (1.3)$$

with

$$\hat{H}_{SO} = \frac{\hbar}{4m^2c^2} (\nabla \mathcal{U} \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}}. \quad (1.4)$$

Due to both the linear  $\hat{\mathbf{p}}$  term and the Pauli matrix  $\sigma_y$ ,  $\hat{H}_{SO}$  is not real. This has strong consequences, in particular for evanescent waves where the effective Hamiltonian matrix can even be non-Hermitian.<sup>2</sup> Following the approach developed by Hoai Nguyen *et al.*,<sup>3</sup> it is convenient to express the full Hamiltonian, including the SOI terms, as an effective Hamiltonian which consists of a momentum-operator  $\hat{\mathbf{p}}$  power series expansion: for instance, in addition to the kinetic energy, quadratic in  $\hat{\mathbf{p}}$ , the SOI may provide leading terms that are linear and cubic in  $\hat{\mathbf{p}}$ , respectively, known as the Bychkov-Rashba<sup>4-6</sup> and Dresselhaus terms.<sup>7</sup> In three-dimensional III-V semiconductors, the Dresselhaus terms are usually expressed through the D'yakonov-Perel (DP) field.<sup>8,9</sup> Then, since the SOI potential is not real, it is necessary to consider a more general definition of the probability current  $\mathbf{J}$ . Taking into account interactions that involve higher-order polynomial terms in the Hamiltonian, we have to deal with an effective Hamiltonian of order  $n$ . This general description applies to holes in valence bands as well as electrons in conduction bands.

Furthermore, an open question, strictly linked to the one above, concerns the spin current (SC), whose standard definition<sup>10,11</sup> has been extensively applied to study spin transport and dynamics,<sup>12-20</sup> spin-polarized tunneling phenomena,<sup>21-23</sup> and the spin-Hall effect.<sup>24-28</sup> However, in semiconductor physics which provides paradigmatic systems for spintronics, it is known that the SC standard definition can be suitably applied to two-dimensional systems with Rashba SOI, but fails to describe spin-dependent transport phenomena in bulk cubic semiconductors, where the SOI induces a DP term in the conduction band. The existence of extra current or extra spin-current terms was pointed out in Ref. 29, where a lengthy but explicit calculation was performed up to the fourth order. More recently, Drouhin *et al.*<sup>30</sup> have proposed a compact expression of the probability-current and SC operators up to the third order; such a modified definition is mandatory to obtain a consistent treatment of tunneling phenomena through GaAs-like semiconductor barriers. Observe that, as pointed out by Rashba in Ref. 10, there are still concerns because a complete theory of spin transport currents has not been formulated yet.

In this paper, we present a systematic construction of the probability-current operator  $\hat{\mathbf{J}}$ , based on an effective Hamiltonian written as a  $\hat{\mathbf{p}}$  power series expansion. We show the relation between the Hermitian velocity operator  $\hat{\mathbf{v}}$  and  $\hat{\mathbf{J}}$ , revealing the simple structure of the extra terms. This procedure yields easy and compact calculations and leads to physically intuitive expressions. The current operator can subsequently be used to build the SC operator  $\delta\hat{\mathbf{J}}$ . Recently, Shi *et al.*<sup>31</sup> have proposed an alternative spin-current operator, satisfying the continuity equation, that they state supports important conclusions concerning conservation of spin currents,<sup>28,32,33</sup> but which relies on several nonexplicit assumptions. Their results are reanalyzed in the present framework.

The layout of this paper is as follows: In Sec. II, we give a general construction of current operators and a derivation of local properties. In Sec. III, we introduce a general Hamiltonian  $\hat{H}^{(n)}$  as an  $n$ th-degree homogeneous function of momentum-operator coordinates; we consistently derive the velocity operator and we show that a proper symmetrization yields the Hermitian current operator  $\hat{\mathbf{J}}$ . In Sec. IV, we show how to deduce the spin-current operator  $\delta\hat{\mathbf{J}}$ .

## II. GENERAL DEFINITION OF CURRENT OPERATORS

Generally speaking, a current operator is defined with respect to a conservation law: Considering the density  $\rho$  of a physical quantity, we need to satisfy the continuity equation related to the current  $\mathbf{J}$ , defining a source term  $G$ , so that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = G. \quad (2.1)$$

It is well known that this decomposition is not unique. Let us consider a linear operator  $\hat{A}$  that does not explicitly depend on time and acts over a generic state  $\psi$ . In the following, we adopt the notations  $(\phi|\psi) = \phi^\dagger \psi$  and  $(\hat{A})_\psi = (\psi|\hat{A}|\psi) = \psi^\dagger \hat{A} \psi$ . The general Schrödinger problem reads

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{\mathcal{H}} \psi, \quad (2.2)$$

where  $\hat{\mathcal{H}}$  may be any Hamiltonian. For example,  $\hat{\mathcal{H}}$  may be equal to  $\hat{H}$  [defined in Eq. (1.3)] or to  $\hat{H}_{\text{eff}}$  [defined below in Eq. (3.1)]. We explicitly develop the derivative of  $(\hat{A})_\psi$  with respect to time:

$$\frac{\partial}{\partial t} (\hat{A})_\psi = \frac{\partial}{\partial t} (\psi^\dagger \hat{A} \psi) = \left( \frac{\partial}{\partial t} \psi^\dagger \right) \hat{A} \psi + \psi^\dagger \hat{A} \left( \frac{\partial}{\partial t} \psi \right), \quad (2.3)$$

and with the help of Eq. (2.2) we obtain

$$\begin{aligned} \frac{\partial}{\partial t} (\hat{A})_\psi &= -\frac{1}{i\hbar} (\hat{\mathcal{H}} \psi)^\dagger \hat{A} \psi + \frac{1}{i\hbar} \psi^\dagger \hat{A} (\hat{\mathcal{H}} \psi) \\ &= \frac{1}{i\hbar} [\psi^\dagger \hat{A} \hat{\mathcal{H}} \psi - (\hat{\mathcal{H}} \psi)^\dagger \hat{A} \psi]. \end{aligned} \quad (2.4)$$

If  $\hat{A}$  is a Hermitian *matrix* (the elements of which are complex numbers, not differential operators),

$$(\hat{\mathcal{H}} \psi)^\dagger \hat{A} \psi = (\psi^\dagger \hat{A} \hat{\mathcal{H}} \psi)^*, \quad (2.5)$$

so that we can rewrite Eq. (2.4) in a more suitable way, which is the local form of Ehrenfest's theorem:

$$\frac{\partial}{\partial t} (\hat{A})_\psi = \frac{2}{\hbar} \text{Im} (\psi^\dagger \hat{A} \hat{\mathcal{H}} \psi). \quad (2.6)$$

The integration over the whole space leads to the well-known Ehrenfest theorem, whose global form is valid for any (possibly differential) Hermitian operator  $\hat{A}$ :

$$\begin{aligned} \frac{d}{dt} \langle \hat{A} \rangle_\psi &= \frac{1}{i\hbar} [\langle \psi | \hat{A} \hat{\mathcal{H}} | \psi \rangle - \langle \hat{\mathcal{H}} \psi | \hat{A} | \psi \rangle] \\ &= \frac{1}{i\hbar} \langle \psi | [\hat{A}, \hat{\mathcal{H}}] | \psi \rangle. \end{aligned} \quad (2.7)$$

We can write

$$\frac{\partial}{\partial t} (\hat{A})_\psi = \frac{1}{\hbar} \text{Im} (\psi^\dagger \{\hat{A}, \hat{\mathcal{H}}\} \psi) + \frac{1}{\hbar} \text{Im} (\psi^\dagger [\hat{A}, \hat{\mathcal{H}}] \psi) \quad (2.8)$$

with  $\{\hat{a}, \hat{b}\} = \hat{a} \hat{b} + \hat{b} \hat{a}$ , and, by integration over the whole space, we get

$$\int d^3 r \text{Im} (\psi^\dagger \{\hat{A}, \hat{\mathcal{H}}\} \psi) = 0. \quad (2.9)$$

The time derivative of  $(\hat{A})_\psi$  can be seen as composed of two parts, concerning two different physical processes: we

recognize in Eq. (2.8) the divergence of the current  $\mathbf{J}_A$  and the source term  $G$  associated with  $\mathbf{J}_A$ :

$$\begin{aligned} \nabla \cdot \mathbf{J}_A &= -\frac{1}{\hbar} \text{Im} (\psi^\dagger \{\hat{A}, \hat{\mathcal{H}}\} \psi) \\ &= -\frac{1}{\hbar} \text{Im} (\psi^\dagger \{\hat{A}, \hat{\mathcal{H}} - \mathcal{U}\} \psi), \end{aligned} \quad (2.10)$$

where the contribution of any Hermitian potential  $\mathcal{U}(\mathbf{r})$  vanishes when taking the imaginary part of the anticommutator, and

$$G = \frac{1}{\hbar} \text{Im} (\psi^\dagger [\hat{A}, \hat{\mathcal{H}}] \psi). \quad (2.11)$$

The above procedure has two advantages: first, we have expressed in a general form all the quantities entering Eq. (2.1) through commutators and anticommutators; then we have related the current expression directly to the local properties of its corresponding operator. Symmetry properties of this current operator are discussed in Appendix A. It has to be noted that it is always possible to include the source term  $G$  in the form of a current  $\mathbf{J}_G$ ,  $G = \nabla \cdot \mathbf{J}_G$  so that the conservation equation becomes

$$\frac{\partial}{\partial t} (\hat{A})_\psi + \nabla \cdot (\mathbf{J}_A - \mathbf{J}_G) = \frac{\partial}{\partial t} (\hat{A})_\psi + \nabla \cdot \mathcal{J} = 0, \quad (2.12)$$

where  $\mathcal{J} = \mathbf{J}_A - \mathbf{J}_G$  is divergence-free in the steady-state regime. For instance, if we look for  $\mathbf{J}_G = \nabla U_G$ , the potential  $U_G$  is a solution of the Laplacian problem  $\Delta U_G = G$ . Obviously, adding to the current a term proportional to the curl of any vector field would not affect the result. Equation (2.9) shows that the flux of  $\mathbf{J}_A$  over the boundary of the whole system, which is a closed system, is zero. At this stage, the boundary conditions on a subsystem are not under control.

## III. PROBABILITY CURRENT OF AN EFFECTIVE HAMILTONIAN

### A. Formulation of the general $n$ th-order Hamiltonian

Considering *effective* Hamiltonians, which are valuable tools to tackle a number of practical problems, we deal with general expressions given by momentum series expansions, e.g., constructed from the energy expressed as a wave-vector-component series expansion after the substitution  $\{k \rightarrow -i\nabla\}$ . We write the effective Hamiltonian  $\hat{H}_{\text{eff}}$  as follows:

$$\hat{H}_{\text{eff}} = \hat{H}_{\mathbf{p}} + V(\mathbf{r}), \quad (3.1)$$

where  $V(\mathbf{r})$  may be the potential of a single barrier or that of a superlattice; for example,  $\hat{H}_{\mathbf{p}}$  is such that

$$\hat{H}_{\mathbf{p}} = \sum_n \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1,\dots,n}} c_{l(1),l(2),\dots,l(n)} \hat{p}_{l(1)} \cdots \hat{p}_{l(n)} = \sum_n \hat{H}^{(n)}, \quad (3.2)$$

where  $\hat{p}_{l(k)}$  is the momentum operator associated with the  $l(k)$  Cartesian coordinate and where  $c_{l(1),\dots,l(n)}$  are Hermitian matrices which commute with  $\hat{\mathbf{p}}$  and which are invariant under permutation of the subscripts. The abstract form of Eq. (3.2) allows us to perform easy calculations.

Formally, we perform the identification

$$\underbrace{c_x \cdots c_x}_\alpha \underbrace{c_y \cdots c_y}_\beta \underbrace{c_z \cdots c_z}_\gamma = \underbrace{c_x \cdots c_x}_\alpha, \underbrace{y \cdots y}_\beta, \underbrace{z \cdots z}_\gamma, \quad (3.3)$$

where  $\alpha$ ,  $\beta$ , and  $\gamma$  are integers. We obtain

$$\widehat{H}^{(n)} = (c_x \widehat{p}_x + c_y \widehat{p}_y + c_z \widehat{p}_z)^n. \quad (3.4)$$

Given Eqs. (3.2), (3.3), and (3.4), let us note that only terms such as  $c_{xx}$  or  $c_{xy}$  (for  $n = 2$ ) are meaningful, a term such as  $c_x$  being only a trick in the calculation.

Alternatively, one can write

$$\widehat{H}^{(n)} = \sum_{\alpha+\beta+\gamma=n} c^{\alpha\beta\gamma} \widehat{p}_x^\alpha \widehat{p}_y^\beta \widehat{p}_z^\gamma \quad (3.5)$$

with

$$c^{\alpha\beta\gamma} = \frac{n!}{\alpha! \beta! \gamma!} c_x^\alpha c_y^\beta c_z^\gamma. \quad (3.6)$$

The velocity operator can be obtained through the relation<sup>1</sup>

$$\widehat{\mathbf{v}} = \frac{i}{\hbar} [\widehat{H}_{\text{eff}}, \widehat{\mathbf{r}}] = \frac{\partial \widehat{H}_{\text{eff}}}{\partial \widehat{\mathbf{p}}}. \quad (3.7)$$

Using Eqs. (3.3)–(3.6), we find that its  $j$ th Cartesian component  $\widehat{v}_j^{(n)}$  ( $j = x, y, z$ ) is

$$\widehat{v}_j^{(n)} = \frac{\partial \widehat{H}^{(n)}}{\partial \widehat{p}_j} = n c_j (c_x \widehat{p}_x + c_y \widehat{p}_y + c_z \widehat{p}_z)^{n-1}. \quad (3.8)$$

Note that, introducing the scalar product between the momentum  $\widehat{\mathbf{p}}$  and the velocity operator  $\widehat{\mathbf{v}}^{(n)}$ , we have

$$\widehat{p}_x \widehat{v}_x^{(n)} + \widehat{p}_y \widehat{v}_y^{(n)} + \widehat{p}_z \widehat{v}_z^{(n)} = n (c_x \widehat{p}_x + c_y \widehat{p}_y + c_z \widehat{p}_z)^n = n \widehat{H}^{(n)}, \quad (3.9)$$

or

$$\widehat{\mathbf{p}} \cdot \widehat{\mathbf{v}}^{(n)} = n \widehat{H}^{(n)}, \quad (3.10)$$

so that  $\widehat{H}_{\text{eff}}$  is simply related to the velocity operator,

$$\widehat{H}_{\text{eff}} \psi = \left( \widehat{\mathbf{p}} \cdot \sum_n \frac{1}{n} \widehat{\mathbf{v}}^{(n)} \right) \psi + V \psi = E \psi. \quad (3.11)$$

This form allows one a straightforward extension of the Bendaniel and Duke procedure<sup>34</sup> to derive boundary conditions at interfaces.<sup>35</sup>

Now, after Eq. (3.8), it is useful to introduce the Hermitian symmetrized velocity operator

$$\begin{aligned} \widehat{\mathbf{v}}_j^{(n)}(\mathbf{r}_0) &= \frac{n}{2} \sum_{l \in \{x, y, z\}, k=1, \dots, n-1} c_{j,l(1), \dots, l(n-1)} \\ &\times [\delta_{\mathbf{r}_0} \widehat{p}_{l(1)} \cdots \widehat{p}_{l(n-1)} + \widehat{p}_{l(1)} \cdots \widehat{p}_{l(n-1)} \delta_{\mathbf{r}_0}], \end{aligned} \quad (3.12)$$

where  $\delta_{\mathbf{r}_0} = \delta(\mathbf{r} - \mathbf{r}_0)$  is the Dirac distribution. The velocity at the point  $\mathbf{r}_0$  is  $\langle \psi | \widehat{\mathbf{v}}_j^{(n)}(\mathbf{r}_0) | \psi \rangle$ . In Appendix B, we show that performing the proper symmetrization according to the rule defined in Eq. (3.14) yields a probability-current operator that,

for the  $j$ th Cartesian component, reads

$$\widehat{\mathbf{J}}_j(\mathbf{r}_0) = \sum_n \widehat{\mathbf{J}}_j^{(n)}(\mathbf{r}_0), \quad (3.13)$$

$$\begin{aligned} \widehat{\mathbf{J}}_j^{(n)}(\mathbf{r}_0) &= \sum_{l \in \{x, y, z\}, k=1, \dots, n-1} c_{j,l(1), \dots, l(n-1)} [\delta_{\mathbf{r}_0} \widehat{p}_{l(1)} \cdots \widehat{p}_{l(n-1)} \\ &+ \widehat{p}_{l(1)} \delta_{\mathbf{r}_0} \cdots \widehat{p}_{l(n-1)} + \cdots + \widehat{p}_{l(1)} \cdots \widehat{p}_{l(n-1)} \delta_{\mathbf{r}_0}]. \end{aligned} \quad (3.14)$$

We must verify that the divergence of the current, calculated with the operator defined by Eq. (3.14), satisfies the conservation equation for the density of probability [Eq. (2.10) when  $\widehat{A}$  is the identity]. It is straightforward to show (Appendix B) that the divergence of the probability current can be written as

$$\begin{aligned} \nabla \cdot \mathbf{J} &= \sum_n \nabla \cdot \mathbf{J}^{(n)} \\ &= -\frac{2}{\hbar} \text{Im} \sum_n \sum_{j \in \{x, y, z\}} \sum_{l \in \{x, y, z\}, k=1, \dots, n-1} \\ &\times (\psi | \widehat{p}_j \widehat{p}_{l(1)} \cdots \widehat{p}_{l(n-1)} c_{j,l(1), \dots, l(n-1)} | \psi). \end{aligned} \quad (3.15)$$

Thus we recover all the terms of Eq. (2.10), which proves that Eq. (3.14) yields a correct definition of the current operator. Such a definition of  $\widehat{\mathbf{J}}$  provides an unambiguous and general tool for evaluating the probability current.

For  $n \geq 3$ , the comparison between the Hermitian symmetrized velocity operator and the current operator [see Eqs. (3.12) and (3.14)] clearly shows that  $\widehat{\mathbf{J}}_j^{(n)}(\mathbf{r}_0)$  contains  $n - 2$  extra terms, which are straightforwardly obtained from  $\partial \widehat{H}_{\text{eff}} / \partial \widehat{\mathbf{p}}$ . For instance, with  $\widehat{H}_{\text{eff}} \equiv \widehat{p}^n$ , we have  $\partial \widehat{H}_{\text{eff}} / \partial \widehat{\mathbf{p}} \equiv n \widehat{p}^{n-1}$ , so that  $\widehat{\mathbf{v}}^{(n)}(\mathbf{r}_0) \equiv (n/2)(\delta_{\mathbf{r}_0} \widehat{p}^{n-1} + \widehat{p}^{n-1} \delta_{\mathbf{r}_0})$ , whereas  $\widehat{\mathbf{J}}^{(n)}(\mathbf{r}_0) \equiv (\delta_{\mathbf{r}_0} \widehat{p}^{n-1} + \widehat{p} \delta_{\mathbf{r}_0} \widehat{p}^{n-2} + \cdots + \widehat{p}^{n-1} \delta_{\mathbf{r}_0})$ . As shown in Ref. 3, these extra terms are especially important for evanescent waves and they have deep consequences for boundary conditions at semiconductor tunnel junctions.<sup>35</sup> Note that, up to the third order, Eq. (3.14) can be written in the simple and intuitive form derived in Ref. 30:

$$\begin{aligned} \widehat{\mathbf{J}}_j(\mathbf{r}_0) &= \delta_{\mathbf{r}_0} a_j + (\delta_{\mathbf{r}_0} \widehat{\mathbf{p}} + \widehat{\mathbf{p}} \delta_{\mathbf{r}_0}) \cdot \underline{b}_j \\ &+ (\delta_{\mathbf{r}_0} \widehat{\mathbf{p}} \widehat{\mathbf{p}}^t + \widehat{\mathbf{p}} \delta_{\mathbf{r}_0} \widehat{\mathbf{p}}^t + \widehat{\mathbf{p}} \widehat{\mathbf{p}}^t \delta_{\mathbf{r}_0}) : \underline{c}_j, \end{aligned} \quad (3.16)$$

where we have kept the notations of Ref. 30, i.e.,  $\widehat{H}^{(1)} = \sum_j a_j \widehat{p}_j$ ,  $\widehat{H}^{(2)} = \sum_{j,k} b_{jk} \widehat{p}_j \widehat{p}_k$ , and  $\widehat{H}^{(3)} = \sum_{j,k,l} c_{jkl} \widehat{p}_j \widehat{p}_k \widehat{p}_l$ , with  $j, k, l = x, y$ , or  $z$ . Then,  $\underline{b}_j$  is a vectorial operator of components  $(\underline{b}_j)_k = b_{jk}$ , and  $\underline{c}_j$  is a second-order symmetric tensorial operator of components  $[\underline{c}_j]_{kl} = c_{jkl}$ . The notation “:” refers to the generalized double-dot product defined by  $\widehat{\mathbf{p}} \widehat{\mathbf{p}}^t : \underline{c}_j = \sum_{kl} p_k p_l c_{jkl}$ .

#### IV. SPIN CURRENT

Equation (3.14) provides a general and symmetrized definition of the probability-current operator. The spin-current operator  $\widehat{\mathbf{J}}_{\mathbf{u}}$  in a direction defined by the unit vector  $\mathbf{u}$  is obtained by taking  $\widehat{A} = \widehat{\sigma}_{\mathbf{u}}$ , the Pauli operator along the  $\mathbf{u}$  direction. It is shown in Appendix B that, as in Ref. 30, the  $j$ th Cartesian component of the spin-current operator is obtained from the  $j$ th component of the probability-current operator after the substitution

$$c_{j,l(1), \dots, l(n)} \rightarrow \frac{1}{2} \{ \widehat{\sigma}_{\mathbf{u}}, c_{j,l(1), \dots, l(n)} \}. \quad (4.1)$$

Because the spin current may be not conserved, there exist source terms

$$G = \frac{1}{\hbar} \text{Im} (\psi^\dagger [\widehat{\sigma}_u, \widehat{\mathcal{H}}] \psi). \quad (4.2)$$

Shi *et al.*<sup>31</sup> have proposed to build a conservative spin current. It is interesting to redo their derivation in the above framework, which has the advantage of putting together the results of Refs. 29 and 31. Shi *et al.* observe that it might often happen that

$$\int_{\mathbb{V}} d^3r G = 0, \quad (4.3)$$

where the integration is performed over the volume of the system ( $\mathbb{V}$ ). Then

$$\int_{\mathbb{V}} d^3r G = \int_{\mathbb{V}} d^3r \nabla \cdot \mathbf{J}_G = \int_{\mathbb{S}} \mathbf{J}_G \cdot d\mathbf{s} = 0, \quad (4.4)$$

where the volume integral is changed into a surface integral through Ostrogradski's theorem (here  $\mathbb{S}$  is the surface limiting  $\mathbb{V}$  and  $d\mathbf{s}$  is the surface element oriented along the normal to  $\mathbb{S}$ ). Such a relation is obviously satisfied provided that  $\mathbf{J}_G \cdot d\mathbf{s} = 0$ , i.e., provided that  $\mathbf{J}_G$  is a tangential vector to  $\mathbb{S}$ , which is physically reasonable.<sup>36</sup> Shi *et al.* further assume that  $\mathbf{J}_G$  "is a material property that should vanish outside the sample," which is a more restrictive hypothesis. Anyway, let us assume that  $\mathbf{J}_G = \mathbf{0}$  at the surface  $\mathbb{S}$ . Following Shi *et al.*'s calculation, it is straightforward to show, after partial integration where the boundary contribution cancels, that

$$\int dy dz dx x \left( \frac{\partial J_{G,x}}{\partial x} + \frac{\partial J_{G,y}}{\partial y} + \frac{\partial J_{G,z}}{\partial z} \right) = - \int d^3r J_{G,x}, \quad (4.5)$$

where  $J_{G,x}$ ,  $J_{G,y}$ , and  $J_{G,z}$  are the Cartesian components of  $\mathbf{J}_G$ . Then

$$\begin{aligned} \int d^3r \mathbf{J}_G &= - \int d^3r \mathbf{r} \nabla \cdot \mathbf{J}_G = - \int d^3r \mathbf{r} G \\ &= - \frac{1}{\hbar} \int d^3r \mathbf{r} \text{Im} (\psi^\dagger [\widehat{A}, \widehat{\mathcal{H}}] \psi) \\ &= - \frac{1}{\hbar} \int d^3r \text{Im} (\psi^\dagger \mathbf{r} [\widehat{A}, \widehat{\mathcal{H}}] \psi). \end{aligned} \quad (4.6)$$

It is easy to check that, provided that  $[\widehat{A}, \mathbf{r}] = 0$  (which is the case for the spin current where  $\widehat{A} = \widehat{\sigma}_u$ ),

$$\mathbf{r} [\widehat{A}, \widehat{\mathcal{H}}] = [\widehat{A} \mathbf{r}, \widehat{\mathcal{H}}] - i \hbar \widehat{\mathbf{v}} \widehat{A}, \quad (4.7)$$

where  $[\mathbf{r}, \widehat{\mathcal{H}}] = i \hbar \widehat{\mathbf{v}}$ . Thus

$$\begin{aligned} \int d^3r \mathbf{J}_G &= - \frac{1}{\hbar} \int d^3r \text{Im} (\psi^\dagger [\widehat{A} \mathbf{r}, \widehat{\mathcal{H}}] \psi) \\ &\quad + \int d^3r \text{Re} (\psi^\dagger \widehat{\mathbf{v}} \widehat{A} \psi) \\ &= - \frac{1}{\hbar} \int d^3r \text{Im} (\psi^\dagger [\widehat{A} \mathbf{r}, \widehat{\mathcal{H}}] \psi) \\ &\quad + \int d^3r \text{Re} \left( \psi^\dagger \frac{\{\widehat{\mathbf{v}}, \widehat{A}\}}{2} \psi \right) \end{aligned} \quad (4.8)$$

$$= - \frac{1}{\hbar} \int d^3r \text{Im} (\psi^\dagger [\widehat{A} \mathbf{r}, \widehat{\mathcal{H}}] \psi) + \int d^3r \widetilde{\mathbf{J}}_A. \quad (4.9)$$

Here,  $\widetilde{\mathbf{J}}_A$  is the canonical current defined as

$$\widetilde{\mathbf{J}}_A = \text{Re} \left( \psi^\dagger \frac{\widehat{\mathbf{v}} \widehat{A} + \widehat{A} \widehat{\mathbf{v}}}{2} \psi \right). \quad (4.10)$$

According to Eq. (2.4), we can write

$$\int d^3r \mathbf{J}_G = \int d^3r \left[ \widetilde{\mathbf{J}}_A - \frac{d(\widehat{A} \mathbf{r})_\psi}{dt} \right]. \quad (4.11)$$

Shi *et al.* define the *effective* current density as  $\overline{\mathbf{J}}_G$ ,

$$\overline{\mathbf{J}}_G = \widetilde{\mathbf{J}}_A - \frac{d(\widehat{A} \mathbf{r})_\psi}{dt}. \quad (4.12)$$

We have the two following relations which define respectively the total current  $\mathcal{J}$  and the *effective* total current  $\overline{\mathcal{J}}$ :

$$\mathcal{J} = \mathbf{J}_A - \mathbf{J}_G, \quad (4.13a)$$

$$\overline{\mathcal{J}} = \mathbf{J}_A - \overline{\mathbf{J}}_G = \frac{d(\widehat{A} \mathbf{r})_\psi}{dt} + (\mathbf{J}_A - \widetilde{\mathbf{J}}_A). \quad (4.13b)$$

Provided  $\mathbf{J}_A - \widetilde{\mathbf{J}}_A = 0$ , i.e., when the canonical and the true currents are set equal (which is justified only for Hamiltonians up to second order in  $\widehat{\mathbf{p}}$ ; see Sec. III), the effective total current becomes  $\overline{\mathcal{J}} = d(\widehat{A} \mathbf{r})_\psi / dt$ , which is Eq. (5) in the paper by Shi *et al.*<sup>31</sup> and also that by Zhang *et al.*,<sup>32</sup> and which is the cornerstone of their further calculations. Thus this relation appears to be derived under special conditions so that it cannot be general. Moreover, the meaning of the so-called effective currents and their relationship with the true currents are not clear [e.g., adding to  $\widetilde{\mathbf{J}}_A$  any term of the form  $\text{Re}(\psi^\dagger \widehat{A} \psi)$ , where  $\widehat{A}$  is any anti-Hermitian linear operator, does not alter the result].

## V. CONCLUSION

We have given a systematic procedure to construct properly symmetrized current operators. Thus, we have obtained a general expression of the probability-current operator up to the  $n$ th order, which clearly shows how the successive terms build up. This generalizes previous results and provides us with a practical tool to perform explicit calculations when dealing with transport problems. The spin-current operator is straightforwardly deduced, with the related expression of the source term. Up to the second order, which includes Bychkov-Rashba Hamiltonians, the current operators coincide with the canonical results. When terms of order larger than 3 are taken into account in the Hamiltonian, extra terms must be included in the current operators. This analysis sheds light on previous discussions as it yields a convenient frame to compare the canonical expressions to the true formulas. The tools we have developed can be applied, for instance, to the holes in the valence band or to the electrons in the conduction band of a III-V semiconductor compound so that they should be important for semiconductor-based spintronics.<sup>37</sup>

## ACKNOWLEDGMENTS

We are grateful to Edouard B. Sonin for valuable discussions. We are indebted to Travis Wade for a careful reading of the manuscript.

**APPENDIX A: SYMMETRY PROPERTIES OF CURRENT OPERATORS**

In Sec. II, Eq. (2.6), we derived the local form of Ehrenfest's theorem for a Hermitian matrix  $\hat{A}$  and deduced the expression of the associated current  $\mathbf{J}_A$ . First, consider the case where  $\hat{A} = \hat{I}$ , where  $\hat{I}$  is the identity, and the quadratic Hamiltonian  $\hat{\mathbf{p}}^2/2m$ . We rewrite Eq. (2.6) as

$$\frac{\partial}{\partial t} |\psi|^2 = -\nabla \cdot \text{Re} \left( \psi^\dagger \frac{\hat{\mathbf{p}}}{m} \psi \right) = -\nabla \cdot \mathbf{J}. \quad (\text{A1})$$

We recover the usual expression for the free-electron probability current

$$\mathbf{J} = \text{Re} \left( \psi^\dagger \frac{\hat{\mathbf{p}}}{m} \psi \right). \quad (\text{A2})$$

Note that

$$\begin{aligned} \frac{\partial}{\partial t} |\psi|^2 &= \frac{1}{i\hbar} \left[ \left( \psi^\dagger \frac{\hat{\mathbf{p}}^2}{2m} \psi \right) - \left( \psi^\dagger \frac{\hat{\mathbf{p}}^2}{2m} \psi \right)^* \right] \\ &= \frac{1}{i\hbar} \left[ \left( \psi^\dagger \frac{\hat{\mathbf{p}}^2}{2m} \psi \right) - (\hat{K}_0 \psi)^\dagger \frac{\hat{\mathbf{p}}^2}{2m} (\hat{K}_0 \psi) \right], \end{aligned} \quad (\text{A3})$$

where  $\hat{K}_0$  is the time-reversal Kramers operator for a spinless particle, which consists of taking the complex conjugate in the  $\mathbf{r}$  representation. Let us check the expression of the current operators we defined under time-inversion symmetry. For this purpose we consider the term [see Eq. (2.10)]

$$\begin{aligned} -2i\hbar \nabla \cdot \mathbf{J}_A &= 2i \text{Im} (\psi^\dagger \{\hat{A}, \hat{H}\} \psi) \\ &= [\psi^\dagger \hat{A} \hat{H} \psi - (\psi^\dagger \hat{A} \hat{H} \psi)^*] \\ &\quad + [\psi^\dagger \hat{H} \hat{A} \psi - (\psi^\dagger \hat{H} \hat{A} \psi)^*]. \end{aligned} \quad (\text{A4})$$

First, look at the term  $\psi^\dagger \hat{A} \hat{H} \psi$ . We find

$$\begin{aligned} (\hat{K} \psi | \hat{A} \hat{H} \hat{K} \psi) &= (\hat{K}_0 \psi | \hat{R}^\dagger \hat{A} \hat{H} \hat{K} \psi) = (\hat{K}_0 \psi | \hat{R}^\dagger \hat{A} \hat{K} \hat{H} \psi) \\ &= -\varepsilon_A (\hat{K}_0 \psi | \hat{R}^\dagger \hat{K} \hat{A} \hat{H} \psi) \\ &= -\varepsilon_A (\hat{K}_0 \psi | \hat{K}_0 \hat{A} \hat{H} \psi) \\ &= -\varepsilon_A (\psi | \hat{A} \hat{H} \psi)^*. \end{aligned} \quad (\text{A5})$$

Here,  $\hat{K} = \hat{R} \hat{K}_0$  is the Kramers operator for a particle with spin  $1/2$ ,  $\hat{R} = -i\sigma_y$  ( $\hat{R}^\dagger = \hat{R}^{-1}$ ), and  $\varepsilon_A = \pm 1$  depending whether  $\hat{A}$  commutes ( $\varepsilon_A = -1$ ) or anticommutes ( $\varepsilon_A = +1$ ) with  $\hat{K}$ ,<sup>38</sup>

$$\hat{K} \hat{A} \hat{K} = \varepsilon_A \hat{A}, \quad \text{i.e.,} \quad \hat{R}^\dagger \hat{A} \hat{R} = \varepsilon_A \hat{A}^*. \quad (\text{A6})$$

Similarly, for the term  $\psi^\dagger \hat{H} \hat{A} \psi$

$$(\hat{K} \psi | \hat{H} \hat{A} \hat{K} \psi) = -\varepsilon_A (\psi | \hat{H} \hat{A} \psi)^*. \quad (\text{A7})$$

Thus, we obtain

$$\begin{aligned} 2i \text{Im} (\psi^\dagger \{\hat{A}, \hat{H}\} \psi) \\ = \psi^\dagger \{\hat{A}, \hat{H}\} \psi + \varepsilon_A (\hat{K} \psi)^\dagger \{\hat{A}, \hat{H}\} (\hat{K} \psi). \end{aligned} \quad (\text{A8})$$

We conclude that the general expression for the current of  $\hat{A}$  is

$$\nabla \cdot \mathbf{J}_A = -\frac{1}{2i\hbar} [\psi^\dagger \{\hat{A}, \hat{H}\} \psi + \varepsilon_A (\hat{K} \psi)^\dagger \{\hat{A}, \hat{H}\} (\hat{K} \psi)], \quad (\text{A9})$$

which gives the behavior of  $\mathbf{J}_A$  upon time reversal,  $\mathbf{J}_A[\psi] = \varepsilon_A \mathbf{J}_A[\hat{K} \psi]$ .

**APPENDIX B: COMPLETE DERIVATION OF THE CURRENT OPERATOR  $\hat{\mathbf{J}}$** 

We are interested in finding the form of the probability current operator  $\hat{\mathbf{J}} = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$  for a Hamiltonian  $\hat{H}_{\text{eff}} = \hat{H}_p + V(\mathbf{r}) = \sum_n \hat{H}^{(n)} + V(\mathbf{r})$  [Eqs. (3.1) and (3.2)]. For a Hamiltonian  $\hat{\mathbf{p}}^2/2m + V(\mathbf{r})$ , it is known<sup>39</sup> that the  $j$ th component of the current operator ( $j = x, y, \text{ or } z$ ) at the point  $\mathbf{r}_0$  is of the shape  $\hat{J}_j^{(2)}(\mathbf{r}_0) = (1/2m)[\delta_{\mathbf{r}_0} \hat{p}_j + \hat{p}_j \delta_{\mathbf{r}_0}]$ ; With the notation of Eqs. (3.1) and (3.2),  $\hat{H}^{(2)} = \sum_{l(k) \in \{x,y,z\}} c_{l(1),l(2)} \hat{p}_{l(1)} \hat{p}_{l(2)}$ ,  $\hat{J}_j^{(2)}(\mathbf{r}_0) = \sum_{l(1) \in \{x,y,z\}} c_{j,l(1)} [\delta_{\mathbf{r}_0} \hat{p}_{l(1)} + \hat{p}_{l(1)} \delta_{\mathbf{r}_0}]$ ,  $c_{l(1),l(2)} = (1/2m) \delta_{l(1),l(2)}$ . The aim of this Appendix is to show that, for a Hamiltonian  $\hat{H}^{(n)}$ , the following form of the  $j$ th component of the probability-current operator  $\hat{\mathbf{J}}^{(n)}$ ,

$$\hat{J}_j^{(n)}(\mathbf{r}_0) = \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} c_{j,l(1), \dots, l(n-1)} [\delta_{\mathbf{r}_0} \hat{p}_{l(1)} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} + \hat{p}_{l(1)} \delta_{\mathbf{r}_0} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} + \cdots + \hat{p}_{l(1)} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} \delta_{\mathbf{r}_0}], \quad (\text{B1})$$

gives back Eq. (2.10) with  $\hat{A}$  being the identity. The Dirac distribution interacts with the mixed powers of the current operator so that the symmetrization procedure used in the construction of  $\hat{J}_j^{(n)}(\mathbf{r}_0)$  provides  $(n-2)$  further summations with respect to the Hermitian symmetrized velocity operator. The two definitions coincide only up to  $n=2$ . When  $n \geq 3$ , the extra terms are crucial in order to satisfy the continuity equation. We evaluate every term over a generic state  $\psi$ ; for example, the second term is of the shape

$$\begin{aligned} \langle \psi | \hat{p}_{l(1)} \delta_{\mathbf{r}_0} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n-1)} | \psi \rangle &= \int d^3 r \psi^\dagger \hat{p}_{l(1)} \delta_{\mathbf{r}_0} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n-1)} \psi \\ &= \int d^3 r (\hat{p}_{l(1)} \psi)^\dagger \delta_{\mathbf{r}_0} \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n-1)} \psi \\ &= [\hat{p}_{l(1)} \psi(\mathbf{r}_0)]^\dagger \hat{p}_{l(2)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n-1)} \psi(\mathbf{r}_0). \end{aligned} \quad (\text{B2})$$

Then the  $j$ th Cartesian component of the probability current for a generic state  $J_j^{(n)}$  can be written as

$$J_j^{(n)} = \langle \psi | \hat{J}_j^{(n)} | \psi \rangle = \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} [\psi^\dagger \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi + \cdots \\ + (\hat{p}_{l(1)} \cdots \hat{p}_{l(k-1)} \psi)^\dagger \hat{p}_{l(k)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi + \cdots + (\hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} \psi)^\dagger c_{j,l(1), \dots, l(n)} \psi]. \quad (\text{B3})$$

From Eq. (B3), we can find the generic divergence term related to the derivative with respect to  $\hat{p}_j$ :

$$\hat{p}_j J_j^{(n)} = \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} [\psi^\dagger \hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi - (\hat{p}_j \psi)^\dagger \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi \\ + (\hat{p}_{l(1)} \cdots \hat{p}_{l(k-1)} \psi)^\dagger \hat{p}_j \hat{p}_{l(k)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi - (\hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(k-1)} \psi)^\dagger \hat{p}_{l(k)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi \\ + (\hat{p}_{l(1)} \cdots \hat{p}_{l(k)} \psi)^\dagger \hat{p}_j \hat{p}_{l(k+1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi - (\hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(k)} \psi)^\dagger \hat{p}_{l(k+1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi \\ + \cdots + (\hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} \psi)^\dagger \hat{p}_j c_{j,l(1), \dots, l(n)} \psi - (\hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} \psi)^\dagger c_{j,l(1), \dots, l(n)} \psi]. \quad (\text{B4})$$

In Eq. (B4) all the terms that have the same order in  $k$  (two consecutive terms except for the first one and the last one) vanish after summation over  $j$ :

$$\sum_{j=\{x,y,z\}} \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} [-(\hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(k-1)} \psi)^\dagger \hat{p}_{l(k)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi \\ + (\hat{p}_{l(1)} \cdots \hat{p}_{l(k)} \psi)^\dagger \hat{p}_j \hat{p}_{l(k+1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi] = 0. \quad (\text{B5})$$

Then the only terms still remaining in the summation are

$$\sum_{j=\{x,y,z\}} \hat{p}_j J_j^{(n)} = \hat{\mathbf{p}} \cdot \mathbf{J}^{(n)} \\ = \sum_{j=\{x,y,z\}} \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} [\psi^\dagger \hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi - (\hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} \psi)^\dagger c_{j,l(1), \dots, l(n)} \psi] \\ = \sum_{j=\{x,y,z\}} \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} 2i \text{Im} \psi^\dagger \hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} \psi. \quad (\text{B6})$$

Now  $\nabla \cdot \mathbf{J}^{(n)} = (i/\hbar) \hat{\mathbf{p}} \cdot \mathbf{J}^{(n)}$  so that

$$\nabla \cdot \mathbf{J}^{(n)} = -\frac{2}{\hbar} \text{Im} \sum_{j=\{x,y,z\}} \sum_{\substack{l(k) \in \{x,y,z\} \\ k=1, \dots, n-1}} (\psi | \hat{p}_j \hat{p}_{l(1)} \cdots \hat{p}_{l(n-1)} c_{j,l(1), \dots, l(n)} | \psi). \quad (\text{B7})$$

Eventually

$$\nabla \cdot \mathbf{J} = \sum_n \nabla \cdot \mathbf{J}^{(n)}.$$

In the more general case of an operator  $\hat{A}$  which verifies  $[\hat{A}, \hat{\mathbf{p}}] = 0$ , it is straightforward to see that  $\hat{\mathbf{J}}_A$  [see Eq. (2.10)] can be constructed through a similar procedure, so that it can be deduced from Eq. (B1), after the substitution

$$c_{j,l(1), \dots, l(n)} \rightarrow \frac{1}{2} [\hat{A}, c_{j,l(1), \dots, l(n)}]. \quad (\text{B8})$$

Special cases of interest are  $\hat{A} = \hat{\sigma}_{\mathbf{u}}$ , the Pauli operator along the  $\mathbf{u}$  direction, which yields the SC operator  $\hat{\delta} \hat{\mathbf{J}}_{\mathbf{u}}$ , and  $\hat{A} = \hat{\pi}_{\uparrow(\downarrow)}$ , the orthogonal projector on the up- (down-) spin state quantized along the  $\mathbf{u}$  axis, which yields the up- (down-) spin-current operator.

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