Spin currents in semiconductors: Redefinition and counterexample

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(Received 7 January 2011; published 29 March 2011)

We show that effective Hamiltonians in solids lead to specific problems when dealing with spin-orbit interaction. We prove that the usual construction, where the velocity operator is simply deduced from the velocity calculated using the Hamilton relation, has a restricted validity and that there is an absolute necessity to modify the standard current-tensor definition. We derive proper symmetrized expressions in the case of a Hamiltonian which has linear and cubic dependence versus momentum components.

DOI: 10.1103/PhysRevB.83.113307

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

The concept of current is of fundamental importance in physics as it governs energy, particle, charge, and spin conservation equations. More specifically, the spin-current (SC) concept is crucial for spintronics. However, its definition in a medium where spin-orbit interaction (SOI) is present remains a subtle point, which gives rise to intense discussions and sometimes epistemological controversies.¹⁻⁴ Let us start from the general form of the Hamiltonian which includes SOI, in the absence of magnetic field,

$$\widehat{H} = \frac{\widehat{\mathbf{p}}^2}{2m} + V + \frac{\hbar}{4m^2c^2} (\nabla V \times \widehat{\mathbf{p}}) \cdot \widehat{\boldsymbol{\sigma}}, \qquad (1)$$

with the usual notations. SOI adds linear $\hat{\mathbf{p}}$ terms to the quadratic kinetic energy so that considering Hamiltonians which have a second-order polynomial $\hat{\mathbf{p}}$ expansion might appear to be a good way to study SOI-related phenomena. In (ferromagnetic) metals, the situation is involved because the electronic structure at the Fermi level is intricate. Semiconductor physics plays a special role in testing the concept of SC in solids because it can provide pure illustrations of quantum mechanics, close to atomic physics, where the whole information of a system can be-often analyticallyobtained (e.g., the wave functions and energy spectrum). In two-dimensional (2D) electron gases, the Rashba Hamiltonian, which adds linear terms to the usual quadratic terms, definitely appears to be a paradigm of spin-orbit coupling effects. In the abstract of a 2003 paper, entitled "Spin currents in thermodynamics equilibrium: The challenge of discerning transport currents, "Rashba¹ states that there are "problems inherent in the theory of transport spin currents driven by external fields" and then starts from the definition which is today commonly accepted: "I use in what follows the standard and physically appealing definition of the SC *tensor* \mathfrak{J}_{ii} ."

In a 2008 paper, Sablikov et al.² reach a similar conclusion. In a detailed analysis relying on thermokinetics arguments, Sun *et al.*³ write that "suggestions have been made in previous papers that one needs to modify the conventional definition of the spin current." But in the framework of their discussion, focused on Rashba SOI, they conclude that "there is no need to modify this conventional definition." To summarize, today the standard definition is to write the (6×6) spin-current tensor as the symmetrized dyadic product $\widehat{\sigma} \widehat{\mathbf{v}}^t$ where the velocity operator $\hat{\mathbf{v}}$ is defined from the Hamilton relation

$$\widehat{\mathfrak{J}} = \frac{1}{2} (\widehat{\mathbf{v}} \widehat{\boldsymbol{\sigma}}^t + \widehat{\boldsymbol{\sigma}} \widehat{\mathbf{v}}^t) \quad \text{with} \quad \widehat{\mathbf{v}} = \frac{\partial \widehat{H}}{\partial \mathbf{p}}, \tag{2}$$

where \widehat{H} is the relevant Hamiltonian. The conceptual difficulty in current definitions is of a general nature and extends to a wide range of physical systems. This can be explained as follows. It is convenient to express the continuity equation for the density ρ of a physical quantity by introducing a current **J** and a source term G,

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J} + G. \tag{3}$$

The point is that the source term is not well defined. It can be modified-an arbitrary part of it can be incorporated in the divergence term-accordingly changing the current definition so that only the current-source couple has a physical meaning.^{4,5} This is analogous to a gauge transformation where different vector- and scalar-potential couples account for a unique physical reality. In spintronics, the source term is referred to as the "spin-transfer torque." Then, the problem of defining both current and source terms in a conservation law is an old problem which was discussed in depth by Feynman in his lecture on electromagnetic-field energy current⁶ and also by De Groot and Mazure in the context of nonequilibrium thermodynamics, for which, however, the second law of thermodynamics provides additional conditions allowing the currents to be uniquely defined.⁷ Even though the argument cannot be used as such in the case of (possibly nondissipative, permanent) quantum currents, there are situations where the equilibrium or steady-state regimes impose boundary conditions that lead to unambiguous identification.

In crystalline solids, the potential V that appears in Eq. (1) is a periodic potential. Through the Bloch theorem, a freeelectron-like Hamiltonian can be recovered by the introduction of an effective mass. Then, the wave-vector (k) dispersion of the energy bands takes the form of a polynomial expression which includes power terms higher than 2. From this dispersion law, an effective Hamiltonian can be built according to the envelope-function theory,⁸ substituting **k** with $\hat{\mathbf{p}}/\hbar$. Dealing with such an effective Hamiltonian enables working with eigenstates described by plane waves but leads to special features because SOI possibly yields momentum terms with a power higher than 2. The use of effective Hamiltonians is crucial when studying nonhomogeneous media (e.g., quantum wells or superlattices) because it is a smart way to take into account the boundary conditions. Therefore, in the present Brief Report, we consider the effective Hamiltonian given by the third-order expansion

$$\hat{H} = H^{(1)} + H^{(2)} + H^{(3)} + U, \qquad (4)$$

where $H^{(1)} = \sum_{j} a_j \hat{p}_j$, $H^{(2)} = \sum_{j,k} b_{jk} \hat{p}_j \hat{p}_k$, and $H^{(3)} = \sum_{j,k,l} c_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l$. The \hat{p}_j , \hat{p}_k , and \hat{p}_l operators are the $\hat{\mathbf{p}}$ components; a_i , b_{ik} , and c_{ikl} (*j*, *k*, and *l* refer to Cartesian coordinates) are (2×2) Hermitian matrices operating in the spin space, invariant under permutation of j, k, and l. The additional perturbing potential U is real.⁹ The linear (first) terms describe the Rashba Hamiltonian, the quadratic (second) terms correspond to the usual kinetic-energy contribution, the cubic (third) terms describe the D'yakonov-Perel' (DP) Hamiltonian¹⁰ (Dresselhaus¹¹ term). Let us point out that the Rashba and DP Hamiltonians are deeply different. Only with some approximations or along special crystallographic directions does the DP Hamiltonian reduce to a form which is a unitary equivalent to the Rashba one.¹² This arises in the situation considered in Ref. 13. Let us emphasize that the third-order expansion of the Hamiltonian covers almost all practical situations in semiconductors, although higher-order terms could be incorporated if needed, without altering the physics discussed in this paper. It was introduced in Ref. 14 to analyze one-dimensional tunneling through evanescent states whose spin properties are determined by the DP field. This calculation is utterly important because it proves that a redefinition of the total probability current is mandatory.

Hereafter, we give a procedure to derive the SC expression relevant to the Hamiltonian given in Eq. (4). A key conclusion is that the standard expression of the SC tensor is correct up to the quadratic terms, which includes Rashba and Klein Hamiltonians,^{1,15} but that, concerning the DP Hamiltonian, a generalized expression has to be used instead. Making use of the results obtained in Ref. 14, we are able to illustrate simply our findings concerning the SC on the concrete case of electron tunneling through GaAs barriers.

First, let us consider the total probability current associated with particle conservation— $\mathbf{J}[\psi]$ originating from the wave function ψ . It will be useful to write $|\psi\rangle = \psi_{\uparrow}|\uparrow\rangle + \psi_{\downarrow}|\downarrow\rangle$ with $\psi_s = \psi_s(\mathbf{r})$, $s = \uparrow$ or \downarrow , $(\psi| = |\psi)^{\dagger}$, and also $(\psi | \varphi) = \psi_{\uparrow}^* \varphi_{\uparrow} + \psi_{\downarrow}^* \varphi_{\downarrow}$. It has been shown in Ref. 14 that the *j* component of $\mathbf{J}[\psi]$ is

$$J_{j}[\psi] = (\psi | a_{j}\psi) + \sum_{k} [(\psi | b_{jk}\hat{p}_{k}\psi) + \text{c.c.}] + \sum_{k,l} [3(\hat{p}_{k}\psi | c_{jkl}\hat{p}_{l}\psi) + \hat{p}_{k}\hat{p}_{l}(\psi | c_{jkl}\psi)], \quad (5)$$

where c.c. means the complex conjugate. The structure of this current can be made more "intuitive" by writing $\mathbf{J}[\psi(\mathbf{r}_0)] = \langle \psi | \hat{\mathbf{J}}(\mathbf{r}_0) | \psi \rangle$, where the *j* component of the (2 × 2) Hermitian current operator¹⁶ $\hat{\mathbf{J}}(\mathbf{r}_0)$ —acting on a spinor—is defined as

$$\widehat{J}_{j}(\mathbf{r}_{0}) = \delta_{\mathbf{r}_{0}}a_{j} + \left(\delta_{\mathbf{r}_{0}}\widehat{\mathbf{p}} + \widehat{\mathbf{p}}\delta_{\mathbf{r}_{0}}\right) \cdot \underline{b}_{j} \\ + \left(\delta_{\mathbf{r}_{0}}\widehat{\mathbf{p}}\widehat{\mathbf{p}}^{t} + \widehat{\mathbf{p}}\delta_{\mathbf{r}_{0}}\widehat{\mathbf{p}}^{t} + \widehat{\mathbf{p}}\widehat{\mathbf{p}}^{t}\delta_{\mathbf{r}_{0}}\right) : \underline{c}_{\underline{=}j}.$$
(6)

In this expression, $\delta_{\mathbf{r}_0} = \delta(\mathbf{r} - \mathbf{r}_0)$ is the Dirac distribution and the notation ": " refers to the double-dot product defined by $M_1: M_2 = \operatorname{Tr}_{\mathbf{r}}(M_1M_2)$, where M_1 and M_2 are arbitrary matrices and $\operatorname{Tr}_{\mathbf{r}}$ is the partial trace calculated over only the space states, e.g., $\widehat{\mathbf{pp}}^t: \underline{c}_j = \sum_{kl} p_k p_l c_{jlk}$. In the space states, the (2×2) Hermitian spin matrix a_j has to be viewed as a scalar operator, \underline{b}_j as a vectorial operator of components $(\underline{b}_j)_k = b_{jk}$, and \underline{c}_j as a second-order symmetric tensorial operator of components $[\underline{c}_j]_{kl} = c_{jkl}$. This current expression differs from the standard one [Eq. (2)]. Indeed, the *j* component of the standard velocity operator is $\hat{v}_j = a_j +$ $\operatorname{Tr}_{\mathbf{r}}[2\underline{b}_j\widehat{\mathbf{p}}^t + 3\underline{c}_j(\widehat{\mathbf{pp}}^t)]$.¹⁴ The simplest use of \hat{v}_j to define $\widehat{\mathbf{J}}_j(\mathbf{r}_0)$ would lead to an equation similar to Eq. (6), where the last term is substituted with $(3/2)(\delta_{\mathbf{r}_0}\widehat{\mathbf{pp}}^t + \widehat{\mathbf{pp}}^t\delta_{\mathbf{r}_0}): \underline{c}_j$.

The SC is the magnetic current originating from the imbalance between the up- and down- spin contributions. Then, it is useful to define separately the up- and down- spin currents and, for that purpose, let us refer to the orthogonal projectors on the basis vectors of the spin space (Hermitian operators commuting with $\hat{\mathbf{p}}$) as π_s , so that $|\psi_s\rangle = \psi_s |s\rangle = \pi_s |\psi\rangle$. Then, it is straightforward to calculate the probability currents associated with the up- and down-spin components of the wave function

$$J_{\mathbf{u},j}[\psi_{s}] = (\psi \mid \pi_{s}a_{j}\pi_{s} \psi) + \sum_{k} [(\psi \mid \pi_{s}b_{jk}\pi_{s} \ \hat{p}_{k}\psi) + \text{c.c.}] + \sum_{k,l} [3(\hat{p}_{k}\psi \mid \pi_{s}c_{jkl}\pi_{s} \hat{p}_{l}\psi) + \hat{p}_{k}\hat{p}_{l}(\psi \mid \pi_{s}c_{jkl}\pi_{s}\psi)],$$
(7)

where **u** is the spin-quantization direction. Any matrix M can be expanded as $M = \pi_{\uparrow} M \pi_{\uparrow} + \pi_{\downarrow} M \pi_{\downarrow} + (\pi_{\uparrow} M \pi_{\downarrow} + \pi_{\downarrow} M \pi_{\uparrow})$. Therefore $J_{\mathbf{u},j}[\psi_{\uparrow}] + J_{\mathbf{u},j}[\psi_{\downarrow}]$ is, in general, *not* equal to the total probability current $J_{\mathbf{u},j}[\psi_{\downarrow}]$, because cross terms involve $(\pi_{\uparrow} M \pi_{\downarrow} + \pi_{\downarrow} M \pi_{\uparrow})$. If M is diagonal, the cross terms vanish. This is the case when \uparrow and \downarrow are eigenstates of \hat{H} and in this special case, we find $J_{\mathbf{u},j}[\psi] = J_{\mathbf{u},j}[\psi_{\uparrow}] + J_{\mathbf{u},j}[\psi_{\downarrow}]$. However, when the quantization direction does not correspond to eigenstates, the meaning of these currents is not obvious. This arises if transport occurs in coupled up- and down-spin channels, and in particular for the DP field in the case of evanescent states when the internal field is not collinear to any real direction.¹⁴

One can properly define the up- and down-spin currents as follows: The principle is to write the conservation equation for the *s*-spin density $\rho_s = |\psi_s|^2$ by projecting the Schrödinger equation on $|\psi_s\rangle$, step by step following the calculation given in Ref. 14, Appendix B. For instance, let us focus on the linear terms in the Hamiltonian: Then $\partial_t \rho_s = -\sum_j \partial_j (\psi | \pi_s a_j \psi)$ $-\frac{1}{i\hbar} \sum_j (p_j \psi | [\pi_s, a_j] \psi)$, with $\partial_j = \partial/\partial x_j$, $x_j = x, y, z$. In general, neither the first term nor the second is real although their sum is. Adding their complex conjugates allows one to construct two real terms: the first one is the divergence of a real quantity that we define as the probability current; we take the second term as the source. This choice is consistent because, if the spin is an eigenstate of the first-order terms in the Hamiltonian (i.e., the spin lies parallel to the corresponding internal field, and a_j is diagonal and commutes with π_s), no spin precession occurs so that the source term must vanish. Then, the source is naturally related to $[a_j, \pi_s]$. Moreover, we will see that this construction leads to the widely used expressions of the probability and spin currents up to first order (i.e., related to $H^{(1)}$ and $H^{(2)}$). The same goes for the quadratic and cubic terms. Eventually, referring to anticommutator as {}, we obtain

$$2J_{\mathbf{u},j}^{s}[\psi] = (\psi|\{\pi_{s},a_{j}\}\psi) + \sum_{k} [(\psi|\{\pi_{s},b_{jk}\}\hat{p}_{k}\psi) + \text{c.c.}] + \sum_{k,l} [3(\hat{p}_{k}\psi|\{\pi_{s},c_{jkl}\}\hat{p}_{l}\psi) + \hat{p}_{k}\hat{p}_{l}(\psi|\{\pi_{s},c_{jkl}\}\psi)], \qquad (8)$$

$$G_{\mathbf{u},s}^{(n)}[\psi] = \frac{1}{\hbar} \operatorname{Im}(\psi | [\pi_s, H^{(n)}] | \psi).$$
(9)

 $G_{\mathbf{u},s}^{(n)}[\psi]$, with n = 1 or 3, refers to the source contribution originating from the linear and cubic terms in the Hamiltonian. To comply with Kramers symmetry, the even-order terms cannot induce any spin splitting: b_{jk} are diagonal matrices and $G_{\mathbf{u},s}^{(2)}[\psi] = 0$. Now, we have $G_{\mathbf{u},\uparrow}^{(n)}[\psi] + G_{\mathbf{u},\downarrow}^{(n)}[\psi] = 0$ and $\mathbf{J}_{\mathbf{u}}[\psi] = \mathbf{J}_{\mathbf{u}}^{\uparrow}[\psi] + \mathbf{J}_{\mathbf{u}}^{\downarrow}[\psi]$. The SC $\delta J_{\mathbf{u},j}[\psi]$ is the difference between the up- and down-spin currents, $\delta J_{\mathbf{u},j}[\psi] = J_{\mathbf{u},j}^{\uparrow}[\psi] - J_{\mathbf{u},j}^{\downarrow}[\psi]$, and the corresponding source terms are $\delta G_{\mathbf{u}}[\psi] = \sum_{n} (G_{\mathbf{u},\uparrow}^{(n)}[\psi] - G_{\mathbf{u},\downarrow}^{(n)}[\psi])$. We obtain

$$2\delta J_{\mathbf{u},j}[\psi] = (\psi | \{\sigma_{\mathbf{u}}, a_j\}\psi) + \sum_{k} [(\psi | \{\sigma_{\mathbf{u}}, b_{jk}\}\hat{p}_{k}\psi) + \text{c.c.}] + \sum_{k,l} [3(\hat{p}_{k}\psi | \{\sigma_{\mathbf{u}}, c_{jkl}\}\hat{p}_{l}\psi) + \hat{p}_{k}\hat{p}_{l}(\psi | \{\sigma_{\mathbf{u}}, c_{jkl}\}\psi)], \quad (10)$$

$$\delta G_{\mathbf{u}}[\psi] = \frac{1}{\hbar} \operatorname{Im}(\psi | [\sigma_{\mathbf{u}}, \hat{H}] | \psi), \qquad (11)$$

where we have used the relation $\sigma_{\mathbf{u}} = \pi_{\uparrow} - \pi_{\downarrow}$. This constitutes a natural extension of the standard definition.¹⁷ Starting from the expression of the *j* component of the total probability current $\mathbf{J}[\psi]$ [Eq. (5)], the SC is straightforwardly obtained by the substitution $a_j \rightarrow a'_j = (1/2)\{\sigma_{\mathbf{u}}, a_j\}, b_{jk} \rightarrow b'_{jk} = (1/2)\{\sigma_{\mathbf{u}}, b_{jk}\}$, and $c_{jkl} \rightarrow c'_{jkl} = (1/2)\{\sigma_{\mathbf{u}}, c_{jkl}\}$. These operators are still Hermitian matrices, invariant under permutation of the subscripts. Thus, the same calculation allows one to write the SC operator in a form similar to Eq. (6). In the case of Rashba splitting, it can easily be checked that these SC and source-term definitions reduce to the standard formulas.⁴ The situation is drastically different in the presence of the DP field.

Let us illustrate the importance of the preceding redefinitions in the particular case of gallium arsenide, for important technological directions. Near the conduction-band edge, the energy is written¹⁰

$$E(\mathbf{k}) = \gamma_c k^2 + \gamma \, \boldsymbol{\chi} \cdot \widehat{\boldsymbol{\sigma}}, \qquad (12)$$

where χ is the DP field, with components $k_x(k_y^2 - k_z^2)$, $k_y(k_z^2 - k_x^2)$, and $k_z(k_x^2 - k_y^2)$, referring to the cubic crystal axes; $\gamma_c(\gamma)$ is a parameter related to the effective mass (DP-field strength).

Along the [110] direction (normal to the cleavage face), taken as the z' axis (unit vector \mathbf{z}'), unidimensional transport can occur for both propagating and evanescent waves.¹⁴ Equation (12) yields the effective Hamiltonian

$$\widehat{H}_{\rm DP} = \frac{\gamma_c}{\hbar^2} \widehat{p}_{z'}^2 + \frac{\gamma}{\hbar^3} \widehat{p}_{z'}^3 \mathbf{e}_{1\overline{1}0} \cdot \widehat{\boldsymbol{\sigma}}, \qquad (13)$$

where $\mathbf{e}_{1\overline{10}}$ is the unit vector along [110], the DP-field direction. It is essential to observe that the evanescent eigenstates of Eq. (13) are *pure* spin states associated with complex wave vectors. As previously pointed out, in that very case, the s-spin current coincides with the probability current carried by ψ_s . At a given energy, there exist four degenerate states, (\mathbf{k}, \uparrow) and (\mathbf{k}^*, \uparrow) for up spin with $\mathbf{k} = (iK + Q)\mathbf{z}'$, where K and Q are real, and their Kramers conjugates for the down spin. As the spin is in an eigenstate, no evolution is expected, no torque will be exerted on it, and no source term should be present. In a tunneling experiment along this direction, transport will take place in two independent channels. Nevertheless, as shown in Ref. 14, up and down spins undergo a different phase shift, which restores spin precession around the complex field. If we consider the state $[(iK + Q)\mathbf{z}', \uparrow]$, the total probability current (charge current) is equal to the up-spin current, which is also the SC. This current has to be conserved as neither charges nor particles can be created inside the material. Let us check this basic conservation rule with the standard SC expression given in Eq. (2). A simple calculation yields

$$\mathfrak{J}_{\mathbf{u},z'}[\psi] = \delta J_{\mathbf{u},z'}[\psi] = -4\frac{\gamma_c}{\hbar}Q|\psi_{\uparrow}|^2, \qquad (14)$$

where we have used the relation $K^2 \simeq (4\gamma_c/\gamma)Q$ [Ref. 14, Eq. (A6)]. Then, we obtain a contradictory result: $\mathfrak{J}_{\mathbf{u},z}[\psi]$ is nonzero and not even divergence-free. This would imply the existence of a nonzero source term which is not physically acceptable and must be excluded. Even a constant current would be nonphysical as the same current would be associated with a vanishingly small wave function for $z' \to +\infty$ and with a diverging wave function for $z' \rightarrow -\infty$. In that case, the SC and the total probability current have to be equal to zero. Contrary to the conclusion given in Ref. 4, there is a need to modify the conventional spin-current definition. Instead, the correct expression for the current [Eq. (7)] yields a zero probability current for an evanescent state along a real-energy line [Ref. 14, Eq. (2.15) and after], as in the case of the usual evanescent wave. It has to be emphasized that a wrong definition of the spin currents implies a wrong definition of the torques. In this tunneling example, if the free-electron probability current were used instead of the correct expression, spurious spin torques would be found. These spurious torques could be "intuitively" related to electron spin precession around the complex DP field. This proves once again that words like "intuitive" or "physical" may be confusing as they rely on quasiclassical pictures.

Finally, let us apply the general relations for the currents and source terms [Eqs. (8)–(10)] in the case of wave functions involving wave vectors with $k_y = 0$. Such solutions are important, in particular because some of them correspond to off-normal tunneling on a [001]-oriented barrier (the GaAs technological surface).¹⁴ Then, the SC components originating from the cubic terms in the Hamiltonian take the simple

form $(\hbar^3/\gamma)\delta J_{\mathbf{z},x}[\psi] = 2 \operatorname{Re}(\hat{p}_x \psi | \hat{p}_z \psi) + (2/3)p_x p_z |\psi|^2$, $\delta J_{\mathbf{z},y}[\psi] = 0$, and $(\hbar^3/\gamma)\delta J_{\mathbf{z},z}[\psi] = |\hat{p}_x \psi|^2 + (1/3)p_x^2 |\psi|^2$. There are simple source terms associated with these SCs: $G_{\mathbf{z},s}^{(3)}[\psi] = (s/\hbar)\operatorname{Re}(\hat{p}_x \hat{p}_z^2 \psi | \sigma_y \psi)$, where s = 1 (-1) for up spin (down spin). By comparison, the standard SC operator [after Eq. (2)] would yield x and z components respectively increased by $(1/3)p_x p_z |\psi|^2$ and $(1/6)p_x^2 |\psi|^2$. The discrepancy in the terms involving $|\psi|^2$ makes evident why evanescent waves, with a rapidly varying modulus, constitute a sensitive probe of the SC properties, whereas propagating plane waves are not.

These results highlight the peculiarities of effective Hamiltonians in crystalline solids. A central achievement is that, up to the second power in the momentum expansion of the Hamiltonian, which includes Rashba Hamiltonians, the commonly accepted SC expression is valid but that, when third-power terms are taken into account as in the DP Hamiltonians along some crystallographic directions, the situation drastically changes. The study of tunneling currents in noncentrosymmetric semiconductors provides one with a unique capability to test the concepts of current. The expression of the SC derived in the present Brief Report, after properly taking into account SOI, paves the way to spinorbit engineering in the ongoing development of spintronics devices.

We are grateful to Emmanuel I. Rashba for his interest. We thank Travis Wade and Federico Bottegoni for a critical reading of the manuscript.

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