Spin rotation, spin filtering, and spin transfer in directional tunneling through non-centrosymmetric semiconductor barriers

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Abstract

We discuss possible tunneling phenomena associated with complex wave vectors along directions where the spin degeneracy is lifted in non-centrosymmetric semiconductors. We show that the result drastically depends on the direction. In the [110] direction, no solution can be calculated in the usual way assuming that the wave function and its derivative are continuous. Conditions that permit one to find physical solutions are discussed and consequences are drawn. As a result, there is no spin filtering in such a direction but the spin undergoes a precession through the barrier with the rotation angle being proportional to the barrier thickness. In a direction close to [001] we find a spin-filter effect in close agreement with the model discussed by Perel et al. [Phys. Rev. B 67, 201304(R) (2003)].

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I. INTRODUCTION

Understanding spin-dependent tunneling through semiconductor barriers is a fundamental problem in semiconductor physics. A description of this coherent process is crucial for spin-subband engineering of semiconductor heterostructures and superlattices. Moreover, spin-dependent tunneling through crystalline barriers has also become a topic of major interest in spintronics. This article thus lies at the interface between general semiconductor physics and spintronics. Regarding semiconductor physics, it has close connections with open problems in the envelope function theory. Harrison studied the problem of heterogeneous materials and introduced the conditions of discontinuity of the envelope function, taking a general viewpoint, well beyond the semiconductor area. A decisive step in semiconductors was performed by BenDaniel and Duke who defined specific discontinuity conditions of the derivative of the envelope function between two media with different effective masses, based on the conservation of the probability current. This approach has been successfully applied to heterostructures by Bastard and has become the standard calculation routine, yielding very accurate energy positions of the energy bands, in perfect agreement with the experimental data. Hereafter, analogously, we deal with periodic lattices which are perturbed by a spin-orbit potential and where, due to the absence of space-inversion symmetry, the spin degeneracy of the bands is lifted through a wave-vector-dependent “exchange” field. We show that the matching conditions of the derivative of envelope function at the boundaries cannot be “as usual”. Thus, the basic tunneling equations are not known.

First of all, dealing with tunneling phenomena requires an accurate knowledge of the energy structure in the forbidden band gap i.e. of the complex band structure of the barrier material. In pioneering articles, Heine and Jones derived general properties of the evanescent states and showed their complexity over 6-dimensional wave-vector space, consisting of complex vectors associating a pure imaginary component to a real - propagating - one. It is often thought that the electrons will tunnel through such complex-wave-vector states as they would do through usual evanescent states (with pure imaginary wave vectors), and this intuitive explanation is probably supported by our familiarity with the tunneling of electrons located in semiconductor side valleys (e.g. in the conduction band of silicon). Hereafter, we deal with spin-dependent tunneling of conduction electrons through a gallium arsenide barrier, a compound with no inversion symmetry. Such processes were investi-
gated by Perel’ et al. in a stimulating article, using the effective mass approximation and under simplifying assumptions; Quite large spin-filter effects were predicted. Although the complex band structure of GaAs was expected to be well known, we have recently found that, in fact, the spin-orbit interaction and the absence of inversion symmetry had never been taken into account simultaneously throughout the Brillouin zone. The evanescent band structure was calculated by several authors. Chang considered semiconductors oriented in the [100], [111], and [110] directions, with space-inversion centers ($O_h$ group) or without space-inversion centers ($T_d$ group), but without taking into account the spin-orbit coupling. Chang and Schulman performed a detailed calculation of the band structure of silicon, which belongs to the $O_h$ group. Schuurmans and t’Hooft studied semiconductors belonging to the $T_d$ group but explicitly discarded terms which lead to odd $k$ terms so that essentially they studied GaAs and AlAs as if they belonged to the $O_h$ group. In Ref. the evanescent band structure in the fundamental gap of GaAs-like III-V semiconductors, including both the spin-orbit coupling and the lack of inversion symmetry, was carefully calculated within a $14 \times 14$ and a $30 \times 30 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian framework. Then it was demonstrated that the evanescent states in the fundamental gap present an original topology, with loops connecting opposite spin states at the center of the Brillouin zone. This very structure has strong consequences for electron tunneling. Here, in order to remove any unnecessary complexity, we start dealing with electrons with a unique effective mass $m$, inside and outside the barrier - an approximation used in numerical applications in Ref. The spin splitting in the barrier is described via the D’yakonov-Perel’ (DP) Hamiltonian. We thus revisit a classic in elementary quantum mechanics - the tunneling of free electrons through a square potential barrier - but in a case where the evanescent states in the barrier are spin split. From general considerations, we derive relevant boundary conditions which are sensitive on the crystallographic direction. We demonstrate that the tunneling process can become rather involved: The case of loop-shaped real-energy lines correspond to wave vectors which have both an imaginary component, which defines the tunneling direction, and an orthogonal real component so that one has to deal, so to say, with a “classical” tunnel effect in the sense where it is possible to recover almost usual tunneling properties - analogous to off-normal tunneling of free electrons - but in a subtle way. In the case of one-dimensional tunneling with a complex (neither real nor purely imaginary) wave vector, the tunnel effect seems to be “anomalous”: A spin precession occurs around a “complex
magnetic field”. We show that the derivative of the envelope function, which is the solution of the Schrödinger equation, undergoes discontinuities at the barrier plane - usually, in semiconductor heterostructures, discontinuities of the derivative arise as a consequence of the different effective masses in the well and in the barrier material and we propose a treatment of heterostructures. After entangling the two spin channels, it is possible to recover a situation which has strong analogy with standard tunneling and where the discontinuity of a “magnetic current” can be viewed as the result of a kinetic-momentum transfer at the barrier interfaces. The spin-orbit-split barrier exerts a torque on the electron spin, similar to spin-torque phenomena in ferromagnetic junctions as predicted by Slonczewski and Berger, but in this latter case, as the barrier is constituted of magnetic material, a spin transfer occurs between the tunneling electrons and the magnetization.

The layout of this paper is as follows: In Sec. II, we give the background relative to the spin splitting and to the conservation of the probability current which will be used afterwards. We show how the spin splitting can lead to complex (not strictly imaginary) wave vectors in the barrier and we analyze the consequences on the probability current. In Sec. III, we study a barrier normal to [110], and in Sec. IV we look in detail at the case of an incident wave whose direction is almost normal to a [001] barrier. A summary is given in Sec. V.

II. BACKGROUND

A. Symmetry

Let us present the notations used throughout the present article (see Fig. 1). $\mathbf{e}$ is a unit vector. The direction of the axes, defined by $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ with respect to crystal axes, will be given in each case. $\mathbf{e}_z$ is normal to the barrier. $\mathbf{e}_z = \mathbf{e}_{110}$ in Sec. III and $\mathbf{e}_z = \mathbf{e}_{001}$ in Sec. IV. We define $\mathbf{k}_I = \xi + \mathbf{q}$, $\mathbf{k}_{II} = \xi + Q + i\mathbf{K}$ ($\xi, \mathbf{q}, Q, \mathbf{K}$ are all real vectors), and $\mathbf{k}_{III} = \xi + \mathbf{q}$. We also introduce the following notations: $\mathbf{p} = x\mathbf{e}_x + y\mathbf{e}_y, \xi = \xi_x \mathbf{e}_x + \xi_y \mathbf{e}_y, \mathbf{q} = q\mathbf{e}_z, Q = Q\mathbf{e}_z, \mathbf{K} = K\mathbf{e}_z, \mathbf{k}_I \cdot \mathbf{r} = k_{III} \cdot \mathbf{r} = \xi x + \xi y + q z, \mathbf{k}_{II} \cdot \mathbf{r} = \xi x + \xi y + (Q + iK) z$. Without spin, the wave function of the incident plane wave and in the barrier should be written as $e^{i(\xi \cdot \mathbf{p} + q z)}$ and $e^{i[\xi \cdot \mathbf{p} + (Q + iK) z]}$ respectively.

To describe the structure of the evanescent states, we use the $\mathbf{k} \cdot \mathbf{p}$ method. In a n-
band model, the energy dispersion curves result from the diagonalization of a \((n \times n)\) \(\mathbf{k} \cdot \mathbf{p}\) Hamiltonian \(\hat{H}\), but \(\mathbf{k}\) is a complex vector so that \(\hat{H}\) is no longer Hermitian and the evanescent states are associated only to real eigenvalues \(E\). To find the energy dispersion curves, we have to solve the secular equation \(\det M(\mathbf{k}) = \det[\hat{H} - E\hat{I}]\), where \(\hat{I}\) is the identity. Because the Hamiltonian is Hermitian when \(\mathbf{k}\) is a real vector, we have the relation \(M(\mathbf{k})^* = M(\mathbf{k}^*)\). Thus, \(\det M(\mathbf{k}^*) = [\det M(\mathbf{k})^*]^* = [\det M(\mathbf{k})]^*\). It follows that \(E_n(\mathbf{k}) = E_{n'}(\mathbf{k}^*)\), where the band indices \(n\) and \(n'\) may or may not refer to the same band. Moreover, Kramers conjugates correspond to the same energy, so that the state associated to \((\mathbf{k}, |\text{up}\rangle)\) and the state associated to \((-\mathbf{k}, |\text{down}\rangle)\) are degenerate. Let us recall that Kramers-conjugate states are obtained by application of \(\hat{K}\), the time reversal operator: \(\hat{K} = -i\sigma_y \hat{K}_0\) where \(\sigma_y\) is the relevant Pauli matrix and \(\hat{K}_0\) is the operation of taking the complex conjugate. Thus in GaAs, the spin degeneracy is lifted and we expect that the four states \([|\mathbf{k}, s\rangle, |\mathbf{k}^*, s'\rangle, |\mathbf{−}k^*, s\rangle, |\mathbf{−}k, s'\rangle]\) be degenerate, \(|s\rangle\) and \(|s'\rangle\) being up-spin states in directions which, generally, are not parallel (Fig. 2). We are going to see a concrete example in Subsec. II B, where \(|s\rangle\) and \(|s'\rangle\) are quantized in the same direction, and in Sec. IV where \(|s\rangle\) and \(|s'\rangle\) are not quantized in the same direction.

### B. Energy levels

In the introduction, we mentioned that the evanescent band structure is deeply altered when the lack of inversion symmetry is taken into account together with the spin-orbit splitting. A particular topology consisting of loops connecting Kramers-conjugate spin states near the zone center was shown along directions of the type \(K[\xi/K, 0, i]\) when the ratio \(\xi/K = \tan \theta\) is fixed. Such loop structure can be expected to arise as it is known that a band cannot stop. Depending on \(\theta\), we obtain the different pictures shown in Fig. 3. The spin vector along a loop is defined by the mean value of the Pauli operator \(\hat{\sigma}\). In the small-\(k\) limit, we get two opposite spin vectors. When going off the zone center, a numerical calculation shows that the two spin vectors rotate to become parallel at the point where the two subbands are connecting. The appearance of these loops is the fingerprint of a strong band mixing of the first conduction band and of the three upper valence bands with remote bands (more precisely with the second conduction band). Indeed, as long as the wave vector remains in some vicinity of \(\Gamma\), the energy levels are well described by the DP Hamiltonian,
where the spin states in the subbands only depend on $\theta$ (see Sec. IV). Observe, in Fig. 3, that - because the extension of the loop tends to zero when $\theta$ tends to $45^\circ$ - the portion of the loops which can be described in this analytical model also has an extension which can become vanishingly small. Hereafter, we stay in the framework of the DP model, which allows analytical calculations.

Throughout the present paper, we take the origin of the energy at the bottom of the conduction band so that the relevant Hamiltonian is written as

$$\hat{H} = \hat{H}_0 + \hat{H}_{DP}$$

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2 = -\gamma_c \nabla^2$$

$$\hat{H}_{DP} = \gamma \chi \cdot \hat{\sigma}$$

(2.1)

where $m$ is the effective mass. $\hat{H}_{DP}$ is the DP Hamiltonian which describes the $k^3$ spin-splitting $\chi = \chi(k) = [\chi_x, \chi_y, \chi_z] = [k_x (k_y^2 - k_z^2), k_y (k_z^2 - k_x^2), k_z (k_x^2 - k_y^2)]$. When $k$ is real, the energy levels are pure spin states, quantized along $\chi$, in the plane perpendicular to $k$. Note that the two eigenvalues of $\chi \cdot \hat{\sigma}$ are opposite, equal to the square roots of $\chi^2 = \chi_x^2 + \chi_y^2 + \chi_z^2$. We designate by $\chi_+ (\chi_-)$ the square roots of $\chi_+ (\chi_-)$ with a positive real part and $\chi_-$ with a negative real part, if relevant). $\chi_+ (\chi_-)$ will be used in Eqs. 2.6 and 2.8

The eigenvalues of $\hat{H}$ are written as $E(k)$.

Inside a finite-width barrier, the incident plane wave $e^{iqz}$ is usually to be replaced by $e^{\pm iKz}$ which corresponds to an imaginary wave vector $\pm iK$.

a) If the incident wave vector $k_I$ is in the [001] direction ($k_I = [0, 0, q]$), the wave vector in the barrier is $k_{II} = [0, 0, \pm iK]$ and the degenerate eigenvalues of $\hat{H}$ are $E(k) = -\gamma_c K^2$ which is the (real) energy $E(k)$ in the forbidden band gap. If $k_I$ is almost in the [001] direction ($k_I = [\xi, 0, q]$ with $\xi \ll q$), $k_{II} = [\xi, 0, \pm iK]$ and the eigenvalues of $\hat{H}$ are $E(k) = -\gamma_c (K^2 - \xi^2) \pm \gamma \xi K \sqrt{K^2 - \xi^2}$ which is the energy $E(k)$ in the forbidden band gap as well.

b) If $k_I$ is in the [110] direction ($k_I = \frac{q}{\sqrt{2}} [110]$), a simple idea would be to take $k_{II} = \pm \frac{iK}{\sqrt{2}} [110]$ which leads to $E(k) = -\gamma_c K^2 \pm i\frac{3}{2} K^3$. This quantity is not real and cannot be an energy $E(k)$. We are therefore led to consider a wave vector such that $k_{II} = \frac{1}{\sqrt{2}} (Q \pm iK)$ [110].

The calculation is given in Appendix A. The resulting band is plotted in Fig. 4, over a very broad energy domain to reveal its general structure. We are only interested in evanescent states located in the forbidden band gap, i.e. states with a small negative energy. For our
purposes, a key point is that, at a given energy, we have exactly the four possible states, the wave vectors of which are \((Q \pm iK)\) with spin \(\uparrow\) and \((-Q \pm iK)\) with spin \(\downarrow\), the latter being obtained from the former through \(\hat{K}\). In short:

\[
E_\uparrow (k) = E_\uparrow (k^*) = E_\downarrow (-k) = E_\downarrow (-k^*)
\] (2.2)

Eq. 2.2 provides us with a concrete example of the ideas developed by Jones who showed that \(E(k) = E(k^*)\). The corresponding four plane waves are \(e^{i(Q \pm iK)} \uparrow\), \(e^{i(-Q \pm iK)} \downarrow\) or \(e^{+Kz}e^{iQz} \uparrow\), \(e^{-Kz}e^{-iQz} \downarrow\) (this is schematically shown in Fig. 5). This leads us to define

\[
\uparrow = e^{iQz} \uparrow \quad \downarrow = e^{-iQz} \downarrow
\] (2.3)

so that the four plane waves write \(e^{\pm Kz} \uparrow\) and \(e^{\mp Kz} \downarrow\).

In the following, \(\uparrow\) and \(\downarrow\) are the up and down spins when the \(\chi\) vector, which plays the role of a magnetic field, lies along a real direction and is taken as quantization axis. When \(\chi\) is not collinear to any real direction, the spin eigenstates are \(\uparrow_k\) and \(\downarrow_k\): In Subsec. IV A we shall see that \(\uparrow_k\) and \(\downarrow_k\) are no longer orthogonal. The implications of a wave vector \(k = Q \pm iK\) in the [110] direction will be considered in detail in Sec. III.

C. Probability current

1. The free-electron probability current

We consider a spin-orbit-split barrier separating two regions where the electron states are described by plane waves and where the potential is taken equal to zero, as shown in Fig. 1. The barrier potential is assumed to be a positive constant. When dealing with tunneling phenomena through crystalline barriers, the wave vector component \(\xi\) parallel to the barrier plane has to be conserved. For an incident plane wave, which has a real wave vector component \(\xi\) parallel to the surface plane, this implies that the imaginary component of the wave vector inside the barrier has to be orthogonal to the barrier plane. Then, the imaginary component of the wave vector inside the barrier defines the tunneling direction. To analyze the tunneling processes, we distinguish two different mechanisms: i) The wave vector has collinear real and imaginary components along the normal to the barrier (we refer to this mechanism as para-type) and ii) The real and imaginary components of the
wave vector in the barrier are orthogonal (we refer to this mechanism as ortho-type). We would point out that a plane wave with the real (imaginary) wave vector \((\xi + Q)\) (resp. \(iK\)) is associated with the "classical" probability current, e.g. calculated for a free electron, \(J_f^f = \frac{\hbar (\xi + Q)}{m}\) (resp. 0). Such currents, with a zero divergence, conserve the local probability in any domain located in the barrier. On the contrary, a plane wave with the wave vector \((\xi + Q) + iK\) is associated to \(J_f^f = e^{-2K \cdot r} \frac{\hbar (\xi + Q)}{m}\) : It looks as if the local probability were to be no longer conserved in a domain located in the barrier, unless \(Q = 0\), because \(\nabla \cdot J_f^f = - (2\hbar/m) (K \cdot Q) e^{-2K \cdot r}\). The case \(Q = 0\), results in a laminar free-electron probability flux. The loops in the complex band structure which have been studied in Ref. 15 correspond to ortho-tunneling, the normal to the barrier plane lying along [001], a direction where the spin splitting is zero. On the contrary, tunneling along the [110] direction, a direction where the DP field is maximum, is a para-process. More precisely, the definition of the free-electron current probability,

\[
J_f^f [\psi] = \text{Re} \left[ \psi^* \frac{\hat{D}}{m} \psi \right] = \frac{\hbar}{m} \text{Im} [\psi^* \nabla \psi]
\]  

(2.4)

is obtained from the conservation of the local probability when the potential in the Schrödinger equation is real.\(^{23}\) Obviously, the equations expressing the conservation of the probability have to be re-examined carefully in our case, where the Hermitian potential is non-real due to the spin-orbit interaction. The detailed derivation of the relevant current operator which allows one to calculate the true currents of probability \(J_{\pm}\) and \(J = J_+ + J_-\) is given in Appendix B. There, it is shown how to extend the usual procedure, which consists to define the velocity \(\hat{v}\) from the relation

\[
\hat{v} = \frac{\partial \hat{H}}{\partial p}
\]  

(2.5)

2. The ortho- and para-processes

Coming back to the specific case of the GaAs-type barrier, let us derive a few basic results and introduce some definitions. The orbital part of the wave function of the conduction band is \(S\) in usual Kane’s notation\(^{24}\) and we write \(\psi_+ = S \uparrow (k)\) and \(\psi_- = S \downarrow (k)\) where \(\uparrow (k) = \uparrow\) [see i) below] or \(\uparrow (k) = \uparrow_k\) [see ii) below] and \(\downarrow (k) = \downarrow [i]\) or \(\downarrow (k) = \downarrow_k\) [ii)]. The corresponding Schrödinger equation is:

\[
i\hbar \frac{\partial \psi_\pm}{\partial t} = \frac{\hat{D}^2}{2m} \psi_\pm + \gamma \chi_\pm (k) \psi_\pm
\]  

(2.6)
i) Ortho-process. Let us assume that $k_{II} = \xi + iK$ (i.e. $\text{Re} k_{II}, \text{Im} k_{II} = 0$, with $\xi \cdot K = 0$) is a possible evanescent state. Because $E = \frac{\hbar^2}{2m} (\xi^2 - K^2)$ is real on a real-energy line, the terms $\chi(\pm k)$ originating from the spin part of the Hamiltonian are also to be real. We follow the usual procedure to derive the expression of the probability current. $\uparrow k$ and $\downarrow k$ are no longer orthogonal but in any case the real spin term disappears so that we obtain

$$\frac{\partial |\psi_\pm|^2}{\partial t} = -\nabla \cdot J^f [\psi_\pm]$$

which is the usual relation for probability conservation. Care has to be taken that the relation $\nabla \cdot J^f [\psi_\pm] = \nabla \cdot J [\psi_\pm]$ does not mean that $J^f [\psi_\pm] = J [\psi_\pm]$. However, in such a case, a number of classical results derived for free electrons will be recovered.

ii) Para-process. In the case of one-dimensional tunneling along the $n$ direction, where $n$ is a unit vector normal to the barrier, which involves a complex wave vector $k = (Q + iK) n$, $\chi(k) = (Q + iK)^3 \chi(n)$, we quantize the spin along the direction of $\chi(n)$ which is a real non-normalized vector. $\chi_\pm(k)$ are no longer real. We follow the same procedure to derive the expression of the probability current and we obtain

$$\frac{\partial |\psi_\pm|^2}{\partial t} = -\nabla \cdot J^f [\psi_\pm] + \frac{2}{\hbar} \gamma \text{Im} \chi_\pm |\psi_\pm|^2$$

These equations could suggest an interpretation in terms of two-channel transport with a generation-recombination rate, analogous to Giant Magnetoresistance phenomena. In such a case, we would classically expect a spin mixing and we will show that, indeed, a formal analogy exists. However, care has to be taken that, at a given $k$, $\psi_+$ and $\psi_-$ do not correspond to the same energy except when $\chi$ is zero.

3. The $[110]$ direction

More specifically, we will deal with electron tunneling along the $[110]$ direction, a direction where the spin splitting is maximum in the real conduction band. On this example, we illustrate the preceding considerations. Let us consider for instance the up-spin channel, where a possible wave vector is $k = (Q + iK) e_{110}$ as shown in Sec. II B, with the wave function

$$\psi_+ (z) = e^{i(Q+iK)z}$$

(2.9)
and the DP field

\[ \chi = \frac{1}{2} (Q + iK)^3 \]  

(2.10)

The free-electron current is

\[ J^f_+ [\psi_+] = \frac{\hbar}{m} \text{Im} \psi^*_+ \nabla \psi_+ = \frac{\hbar Q}{m} e^{-2Kz} \]  

(2.11)

\[ \nabla \cdot J^f_+ [\psi_+] = -\frac{2\hbar}{m} KQ e^{-2Kz} \]  

(2.12)

On a real-energy line (see Eq. [A3])

\[
\frac{\partial |\psi_+|^2}{\partial t} = -\nabla \cdot J_+ [\psi_+] = \frac{2\hbar}{m} KQ e^{-2Kz} + \frac{\gamma}{\hbar} \text{Im} (Q + iK)^3 e^{-2Kz} \\
= \frac{2K}{\hbar} \left[ 2\gamma Q + \frac{1}{2} \gamma (3Q^2 - K^2) \right] e^{-2Kz} = 0
\]

(2.13)

Along the real-energy line, the eigenstates of the Schrödinger equation comply, as expected, with the continuity equation, the current \( J_+ \) being to be identified. Here, it is easy to show that (see Appendix [B])

\[ J_\pm [\psi_\pm] = J^f_+ [\psi_\pm] \pm \frac{\gamma}{2\hbar} \left( 3 \left| \frac{\partial}{\partial z} \psi_\pm \right|^2 - \frac{\partial^2}{\partial z^2} |\psi_\pm|^2 \right) \]  

(2.14)

In the real conduction band, taking \( \psi_\pm = e^{iqz} \), we obtain

\[ J_\pm [e^{iqz}] = \frac{2\gamma c}{\hbar} q \pm \frac{3}{2\hbar} q^2 \frac{\gamma}{\hbar} \partial q \left[ \gamma c q^2 \pm \frac{1}{2} \gamma q^3 \right] = \frac{1}{\hbar} \frac{\partial}{\partial q} E(q) \]  

(2.15)

Concerning an evanescent wave \( \psi_\pm = e^{(K+iQ)z} \), it is easy to check that \( J_\pm [e^{(K+iQ)z}] = 0 \) on a real-energy line.

4. Waves conserving the free-electron probability current

The waves which conserve the free-electron current of probability play a special role: They appear to be "quasi-classical states" which allow us to build solutions yielding intuitive physical interpretations. The waves involved in an ortho-process verify \( \text{Re} \mathbf{k} \cdot \text{Im} \mathbf{k} = 0 \) and we have seen in Sec. [II C 2] that this condition ensures the conservation of \( J^f_+ \). In the case of a para-process, a paradigm being tunneling along [110], \( J^f_+ \) is not conserved in a given spin channel. Therefore, it is necessary to consider an intricated wave function, \( \psi (\mathbf{r}) = \psi_+ (\mathbf{r}) \uparrow + \psi_- (\mathbf{r}) \downarrow = \psi_+ \uparrow \uparrow + \psi_- \downarrow \downarrow = \psi_\uparrow \uparrow + \psi_\downarrow \downarrow \). In the following, we indifferently use the notation \( \psi_+ \) and \( \psi_- \) or \( \psi_\uparrow \) and \( \psi_\downarrow \).
The free-electron probability current is given by \( \mathbf{J}^f \psi = (1/m) \text{Re} \langle \psi^* \hat{\mathbf{p}} \psi \rangle_\sigma \) where the index \( \sigma \) means a summation (partial trace) on the spin or \( \mathbf{J}^f \psi = (1/m) \text{Re} \langle \psi^* \hat{\mathbf{p}} \psi_+ + \psi^* \hat{\mathbf{p}} \psi_- \rangle = \mathbf{J}^f [\psi_+] + \mathbf{J}^f [\psi_-] \). Due to Kramers symmetry, the wave functions in the barrier \( \psi_{II+} \) and \( \psi_{II-} \) can be written

\[
\psi_{II+}(z) = A_2 e^{i(Q+\lambda K)z} + B_2 e^{i(Q-\lambda K)z} \\
\psi_{II-}(z) = \bar{A}_2 e^{i(-Q+\lambda K)z} + \bar{B}_2 e^{i(-Q-\lambda K)z}
\] (2.16)

The free-electron probability current carried by the function of the type \( \phi = (A_2 e^{-Kz} + B_2 e^{Kz}) e^{iQz} \) is (\( \epsilon = \pm 1 \))

\[
\mathbf{J}^f [\phi] = \frac{\hbar}{m} \left[ 2K \text{Im} A_2^* B_2 + \epsilon Q \left( 2 \text{Re} A_2 B_2^* + |A_2|^2 e^{-2Kz} + |B_2|^2 e^{2Kz} \right) \right]
\] (2.17)

In the barrier, let us write \( \Psi_{II} = \Psi_{II+} \uparrow + \Psi_{II-} \downarrow \), so we have

\[
\mathbf{J}^f [\Psi_{II}] = \frac{\hbar}{m} \left\{ 2Q \left[ \text{Re} B_2 A_2^* - \text{Re} \tilde{B}_2 \tilde{A}_2^* \right] + 2K \left[ \text{Im} B_2 A_2^* + \text{Im} \tilde{B}_2 \tilde{A}_2^* \right] + Q \left[ e^{-2Kz} \left( |A_2|^2 - |	ilde{A}_2|^2 \right) + e^{2Kz} \left( |B_2|^2 - |	ilde{B}_2|^2 \right) \right] \right\}
\] (2.18)

We see that the probability current in the barrier is constant if and only if \( |A_2| = |\tilde{A}_2| \), \( |B_2| = |\tilde{B}_2| \). This leads to \( A_2 = \mathcal{A} e^{i\theta_A}, \tilde{A}_2 = \mathcal{A} e^{-i\theta_A}, B_2 = \mathcal{B} e^{i\theta_B}, \) and \( \tilde{B}_2 = \mathcal{B} e^{-i\theta_B} \) where \( \mathcal{A} \) and \( \mathcal{B} \) are two complex numbers. So the general expression of a wave sustaining a constant \( \mathbf{J}^f \) inside the barrier is

\[
\Psi_{II} = \Psi_{II}(z) = \mathcal{A} e^{-Kz} \left[ e^{i\theta_A} \uparrow + e^{-i\theta_A} \downarrow \right] + \mathcal{B} e^{Kz} \left[ e^{i\theta_B} \uparrow + e^{-i\theta_B} \downarrow \right]
\] (2.19)

It is useful to write

\[
\Psi_{II}(z) = \mathcal{A} e^{-Kz} S_{\exp i\theta_A} + \mathcal{B} e^{Kz} S_{\exp i\theta_B}
\] (2.20)

where

\[
S_\lambda = S_\lambda (z) = \lambda \uparrow + \lambda^* \downarrow
\] (2.21)

The Kramers conjugate of \( S_\lambda \) is \( \tilde{S}_\lambda = \hat{K} S_\lambda \) where \( \hat{K} \) is the time reversal transformation. Observe that \( S_\lambda \) and \( \tilde{S}_\lambda \) are eigenstates of the helicity operator \( (\hat{\mathbf{p}} \cdot \hat{\sigma}) \) for the eigenvalue \( \hbar Q \).

Let us look at the spin direction defined by \( S_\lambda \). Recall that the spin quantization direction is along the \( \chi (e_{110}) \) vector. We call \( O_\chi \) the direction parallel to \( \chi (e_{110}) \); \( O_x' \) and \( O_y' \) are
in the $\Pi_\chi$ plane normal to $\chi$ ($e_{110}$). The spin direction is defined via $\langle \sigma_{x'} \rangle$, $\langle \sigma_{y'} \rangle$, $\langle \sigma_{z'} \rangle$. First of all we note that $\langle \sigma_{x'} \rangle = 0$ while $\langle \sigma_{x'} \rangle = 2 \Re \lambda^2$ and $\langle \sigma_{y'} \rangle = -2 \Im \lambda^2$ for $S_{\lambda}(0)$. The spin is in the $\Pi_\chi$ plane. Any spin direction in the $\Pi_\chi$ plane, that we call an *in-plane* direction, can be described by a suited value of $\lambda$. For instance with $\lambda = \exp i \theta_\lambda$, $\langle \sigma_{x'} \rangle = \cos 2 \theta_\lambda$, and $\langle \sigma_{y'} \rangle = -\sin 2 \theta_\lambda$, apart a common factor, $\theta_\lambda$ being the angle between the $Ox'$ axis and the spin direction.

It can be shown that the largest vectorial space consisting of $J^f$-conserving waves at a given energy is $\mathcal{E} = \{ \Psi_{\alpha,\beta} \}$ where

$$\Psi_{\alpha,\beta} = (\alpha A e^{-Kz} + \beta B e^{Kz}) \uparrow + (\alpha^* A e^{Kz} + \beta^* B e^{Kz}) \downarrow$$  \hspace{1cm} (2.22)

with $\alpha$ and $\beta \in \mathbb{C}$. $\mathcal{E}$ is a vectorial space over $\mathbb{R}$, but not over $\mathbb{C}$.

Moreover, the existence of a superposition principle implies that any linear combination with real coefficients of two solutions with a current of probability of a given sign has to be a solution associated to a current of probability of the same sign. This is a strong constraint which is verified over $\mathcal{E}_0 = \{ \Phi_{A,B} \otimes \{ S_{\lambda} \} = \{( A e^{-Kz} + B e^{Kz}) S_{\lambda} \}$, a vectorial subspace of $\mathcal{E}$ (in this subspace $J^f [\Phi_{A,B} S_{\lambda}] = 2 |\alpha|^2 J^f [\Phi_{A,B}]$, or in $\{( \Phi_{A,B} S)_{\lambda,\theta} = \cos \theta \Phi_{A,B} S_{\lambda} + \sin \theta \frac{1}{K} \frac{d}{dz} \Phi_{A,B} (i \hat{S}_\lambda) \}_{\theta}$ - at fixed $\theta$ - which also is vectorial subspace (in this subspace $J^f [(\Phi_{A,B} S)_{\lambda,\theta}] = 2 |\alpha|^2 J^f [\Phi_{A,B} \cos 2\theta]$).

**D. Standard tunneling case**

The standard tunneling case is to be recovered when $\gamma$ is zero, therefore, we build our analysis in close relation with it. A crucial point is that the probability current has to be constant so that $R + T = 1$ where $R$ ($T$) is the reflection (transmission) coefficient.

We shall need the standard (without spin) function $\psi^{(0)}(z)$ defined as:

$$\psi^{(0)}(z) = \begin{cases} 
\psi_I^{(0)}(z) = a_1 e^{iqz} + b_1 e^{-iqz} & (z < 0) \\
\psi_{II}^{(0)}(z) = a_2 e^{-Kz} + b_2 e^{Kz} & (0 < z < a) \\
\psi_{III}^{(0)}(z) = a_3 e^{iqz} & (a < z) 
\end{cases}$$  \hspace{1cm} (2.23)

where $z < 0$, $0 < z < a$, and $a < z$ respectively correspond to the incident wave (index $I$), to the wave in the barrier (index $II$), and to the transmitted wave (index $III$), as illustrated in Fig. 1.
\( \psi^{(0)}(z) \), a \( C^1 \)-function, meets the boundary conditions

\[
\psi^{(0)}(z_0-) = \psi^{(0)}(z_0^+) \quad \text{and} \quad \frac{\partial \psi^{(0)}(z_0-)}{\partial z} = \frac{\partial \psi^{(0)}(z_0^+)}{\partial z}, \quad z_0 = 0 \text{ or } a
\]  

(2.24)

\[
\begin{align*}
\frac{b_1}{a_1} &= \frac{2 (q^2 + K^2) \sinh KA \exp K a \gg 1}{D} \left( \frac{q^2 + K^2}{(q+iK)^2} \right) \\
\frac{a_2}{a_1} &= \frac{2q (q+iK) e^{KA} \exp K a \gg 1}{D} \approx 2 \frac{q}{(q+iK)} \\
\frac{b_2}{a_1} &= \frac{2q (-q+iK) e^{-KA} \exp K a \gg 1}{D} \approx 2 \frac{q (-q+iK)}{(q+iK)^2} e^{-2KA} \\
\frac{a_3}{a_1} &= \frac{4iKq e^{-iqa} \exp K a \gg 1}{D} \approx 4i \frac{qKe^{-iqa}}{(q+iK)^2} e^{-Ka} \\
D &= (q+iK)^2 e^{Ka} - (q-iK)^2 e^{-Ka}
\end{align*}
\]  

(2.25)

The function \( \psi^{(0)}(z) \) is such that the probability current \( \mathbf{J}^f[\psi^{(0)}] \) is constant. The reflection coefficient \( R = |b_1/a_1|^2 \) and the transmission coefficient \( T = |a_3/a_1|^2 \) are such that \( R + T = 1 \).

Also observe that, if we multiply \( \psi^{(0)} \) by any \( C^1 \)-function \( f(r, \uparrow, \downarrow) \), the new function and its derivative are continuous at the interfaces, satisfying the initial boundary conditions. Consider the case where the incident wave is \( e^{iqr} \). If we take \( f(r, \uparrow, \downarrow) = e^{i\xi r} \uparrow \) or \( f(r, \uparrow, \downarrow) = e^{i\xi r} \downarrow \), we obtain a solution to the tunneling problem if, and only if, the incident component \( e^{i(q+\xi)r} \) and the reflected component \( e^{i(-q+\xi)r} \), correspond to the same energy.

III. PARA PROCESS: [110]-ORIENTED BARRIER UNDER NORMAL INCIDENCE

A. General considerations

In the case where the wave vector is parallel to the [110] direction and the \( \hat{H}_{DP} \) Hamiltonian is taken into account, we have seen in Sec. III B that the wave vector is to be of the form \( (\epsilon Q \pm iK) e_{110} \) to get a real eigenvalue (an energy) of the Hamiltonian. But in such case, \( \mathbf{J}^f \) is not conserved (Eq. 2.17) and even not constant inside the barrier, so that the standard calculation routine to find the solution (i.e. the continuity of the wave function and of its derivative) cannot apply.
We could try to build a solution according to the usual procedure, but with a wave in the barrier involving the two spin channels, which can give a constant $J'$ (see Eq. 2.19)

$$
\Psi (z) = \begin{cases} 
\Psi_I (z) &= (A_1 e^{iqz} + B_1 e^{-iqz}) \uparrow + \tilde{B}_1 e^{-iqz} \downarrow \\
\Psi_{II} (z) &= (A_2 e^{-Kz} + B_2 e^{Kz}) \uparrow + \left( \tilde{A}_2 e^{-Kz} + \tilde{B}_2 e^{Kz} \right) \downarrow \\
\Psi_{III} (z) &= A_3 e^{iqz} \uparrow + \tilde{A}_3 e^{iqz} \downarrow 
\end{cases} \quad (3.1)
$$

where $\uparrow$ and $\downarrow$ are defined in Eq. 2.3.

The usual boundary conditions ($C^1$ function) for the down-spin channel for instance yield four equations determining $\tilde{B}_1$, $\tilde{A}_2$, $\tilde{B}_2$, and $\tilde{A}_3$

$$
\tilde{B}_1 = \tilde{B}_2 + \tilde{A}_2 \\
q \tilde{B}_1 = (Q - iK) \tilde{A}_2 + (Q + iK) \tilde{B}_2 \\
\tilde{A}_2 e^{-i(Q-iK)a} + \tilde{B}_2 e^{-i(Q+iK)a} = \tilde{A}_3 e^{iqa} \\
\tilde{A}_2 (Q - iK) e^{-i(Q-iK)a} + \tilde{B}_2 (Q + iK) e^{-i(Q+iK)a} = -\tilde{A}_3 q e^{iqa} \quad (3.2)
$$

They only provide a non trivial solution if the determinant of the system is equal to 0 which gives the relation

$$
(q^2 - Q^2 - K^2) \sinh K a + 2iK q \cosh K a = 0 \quad (3.3)
$$

The only solution is $K = 0$ but it is not relevant to our problem.

**B. Solutions to the tunneling problem**

1. **The constant-$\gamma$ case**

We go back to the Schrödinger equation to determine the proper boundary conditions and, to avoid any unnecessary mathematical complexity, we here assume that $\gamma$ is constant over the three regions. Along the [110] direction, with $\mathbf{k} = (1/\sqrt{2}) k [110]$, the DP Hamiltonian writes

$$
H_{DP} = \gamma_c k^2 \pm \frac{1}{2} \gamma k^3 \quad (3.4)
$$

where the $+$ (resp. $-$) sign applies to the up (down) spin, quantized along the DP field. As usual, we obtain the effective Hamiltonian by substituting $\mathbf{k}$ with $-i \nabla$, i.e. $k$ with $-i \frac{\partial}{\partial z}$.

$$
H_{DP} = -\gamma_c \frac{\partial^2}{\partial z^2} \pm \frac{i}{2} \gamma \frac{\partial^3}{\partial z^3} \quad (3.5)
$$
Thus, we have the two equations

\[
\begin{align*}
-\gamma c \frac{\partial^2}{\partial z^2} + \frac{1}{2} i \gamma \frac{\partial^3}{\partial z^3} & \psi_\uparrow = [E - V(z)] \psi_\uparrow \\
-\gamma c \frac{\partial^2}{\partial z^2} - \frac{1}{2} i \gamma \frac{\partial^3}{\partial z^3} & \psi_\downarrow = [E - V(z)] \psi_\downarrow
\end{align*}
\] (3.6)

where \( V(z) = V \) when \( 0 \leq z \leq a \) and \( V(z) = 0 \) outside. Because the DP Hamiltonian was obtained using the perturbation theory, we will look for a solution to the effective Schrödinger equation to the first order in \( \gamma \) only. Let us consider the up-spin channel: We write

\[
\psi_\uparrow = \psi^{(0)} + \psi^{(1)}_\uparrow
\] (3.7)

where \( \psi^{(0)} \) is the standard function (obtained for \( \gamma = 0 \), and defined by Eq. 2.23). It is a \( C^1 \) function, with a discontinuous second derivative). \( \psi^{(1)}_\uparrow \) is a first-order term in \( \gamma \) so that the Schrödinger equation to the first order writes

\[
-\gamma c \frac{\partial^2 \psi_\uparrow}{\partial z^2} + \frac{1}{2} i \gamma \frac{\partial^3 \psi^{(0)}_\uparrow}{\partial z^3} = [E - V(z)] \psi_\uparrow
\] (3.8)

We integrate this equation from one side of the interface to the other

\[
-\gamma c \left[ \frac{\partial \psi_\uparrow}{\partial z} \right]_{z_0^-}^{z_0^+} + \frac{1}{2} i \gamma \left[ \frac{\partial^2 \psi^{(0)}_\uparrow}{\partial z^2} \right]_{z_0^-}^{z_0^+} = \int_{z_0^-}^{z_0^+} [E - V(z)] \psi_\uparrow dz
\] (3.9)

Then

\[
\lim_{\epsilon \to 0} \left\{ -\gamma c \left[ \frac{\partial \psi_\uparrow}{\partial z} \right]_{z_0^-}^{z_0^+} + \frac{1}{2} i \gamma \left[ \frac{\partial^2 \psi^{(0)}_\uparrow}{\partial z^2} \right]_{z_0^-}^{z_0^+} \right\} = 0
\] (3.10)

Taking the standard function (Eq. 2.23) and referring to the limit at \( z_0 \) inside the barrier and inside the well respectively as \( z_0^B \) and \( z_0^W \), we obtain

\[
\left[ \frac{\partial^2 \psi^{(0)}_\uparrow}{\partial z^2} \right]_{z_0^W} = -q^2 \psi^{(0)}_\uparrow(z_0^W)
\] (3.11)

outside the barrier, and

\[
\left[ \frac{\partial^2 \psi^{(0)}_\uparrow}{\partial z^2} \right]_{z_0^B} = K^2 \psi^{(0)}_\uparrow(z_0^B)
\] (3.12)

inside the barrier. At the interfaces \( \psi^{(0)}(z_0^B) = \psi^{(0)}(z_0^W) = \psi^{(0)}(z_0) \), then

\[
\left[ \frac{1}{2} i \gamma \left( \frac{\partial^2 \psi_\uparrow}{\partial z^2} \right) \right]_{z_0^W} = \frac{1}{2} i \gamma \left( K^2 + q^2 \right) \psi^{(0)}(z_0)
\] (3.13)
This provides us with the jump of the derivative at the interfaces. To the first order in $q/K$

$$
\left[ \frac{\partial \psi}{\partial z} \right]_{z_0}^{z_B} = \frac{1}{2} \frac{\gamma}{\gamma_c} (K^2 + q^2) \psi^{(0)}(z_0) \approx \frac{1}{2} i \frac{\gamma}{\gamma_c} K^2 \psi^{(0)}(z_0) = 2iQ_1 \psi^{(0)}(z_0) \quad (3.14)
$$

after Eq. A9.

Similarly, for a down spin $Q_\downarrow = -Q_\uparrow$, and we have

$$
\left[ \frac{\partial \psi}{\partial z} \right]_{z_0}^{z_W} = 2iQ_1 \psi^{(0)}(z_0) \quad (3.15)
$$

It is worth remarking that this very discontinuity condition was found in a quite different situation, involving Rashba-split quantum wells.\textsuperscript{27}

Now let us assume that $Q_\uparrow = Q$. The wave function constructed from the eigenstates in the three regions is

$$
\psi(z) = \begin{cases} 
\psi_I(z) = A_1 e^{iqz} + B_1(q, K, Q) e^{-iqz} & (z < 0) \\
\psi_{II}(z) = A_2(q, K, Q) e^{-Kz} e^{iQz} + B_2(q, K, Q) e^{Kz} e^{iQz} & (0 < z < a) \\
\psi_{III}(z) = A_3(q, K, Q) e^{iqz} & (a < z)
\end{cases} \quad (3.16)
$$

with the coefficients $B_1(q, K, Q), A_2(q, K, Q), B_2(q, K, Q),$ and $A_3(q, K, Q)$ to be determined.

To the first order in $Q$, the solution can be expanded as

$$
\psi_I(z) = (a_1 e^{iqz} + b_1 e^{-iqz}) + \beta_1 Q e^{-iqz} \\
\psi_{II}(z) = (a_2 e^{-Kz} + b_2 e^{Kz}) e^{iQz} + Q (a_2 e^{-Kz} + b_2 e^{Kz}) e^{iQz} \\
\psi_{III}(z) = a_3 e^{iqz} e^{iQa} + \alpha_3' Q e^{iqz}
$$

with

$$
\beta_1 = \left[ \frac{d B_1(q, K, Q)}{d Q} \right]_{Q=0} \quad (3.18)
$$

$$
\alpha_2 = \left[ \frac{d A_2(q, K, Q)}{d Q} \right]_{Q=0} ; \quad \beta_2 = \left[ \frac{d B_2(q, K, Q)}{d Q} \right]_{Q=0} \quad (3.19)
$$

and

$$
\alpha_3 = \left[ \frac{d A_3(q, K, Q)}{d Q} \right]_{Q=0} \simeq iaa_3 + \alpha_3' \quad (3.20)
$$

We write

$$
\psi = \varphi^S + \varphi^{\hat{S}} \quad (3.21)
$$
where

\[ \varphi^S(z) = \begin{cases} 
\varphi^S_I(z) &= a_1 e^{iqz} + b_1 e^{-iKz} & (z < 0) \\
\varphi^S_{II}(z) &= (a_2 e^{-Kz} + b_2 e^{Kz}) e^{iQz} & (0 < z < a) \\
\varphi^S_{III}(z) &= a_3 e^{iqz} e^{iQa} & (a < z)
\end{cases} \] (3.22)

\[ \varphi^\beta(z) = \begin{cases} 
\varphi^\beta_I(z) &= \beta_1 Q e^{-iQz} & (z < 0) \\
\varphi^\beta_{II}(z) &= Q (\alpha_2 e^{-Kz} + \beta_2 e^{Kz}) e^{iQz} & (0 < z < a) \\
\varphi^\beta_{III}(z) &= \alpha_3' Q e^{iQz} & (a < z)
\end{cases} \] (3.23)

\( \varphi^S \) is a continuous function but its derivative is not. To the first order, its jump at the interfaces is

\[ \left[ \frac{\partial \varphi^S}{\partial z} \right]_{z=B}^{z=W} = iQ \psi_{II}^{(0)}(z_0) \] (3.24)

As we have derived that the jump of the derivative of the wave function \( \psi \) is \( 2iQ \psi_{II}^{(0)}(z_0) \), we deduce that \( \varphi^\beta \) is a continuous function and that the jump of its derivative at the interfaces is

\[ \left[ \frac{\partial \varphi^\beta}{\partial z} \right]_{z=B}^{z=W} = iQ \psi_{II}^{(0)}(z_0) \] (3.25)

This provides us with the four equations which determine the four coefficients \( \beta_1, \alpha_2, \beta_2, \) and \( \alpha_3' \)

\[ \beta_1 - \alpha_2 - \beta_2 = 0 \]
\[ \alpha_2 e^{-Kz} + \beta_2 e^{Kz} - \alpha_3' e^{iQz} = 0 \]
\[ iq \beta_1 - K \alpha_2 + K \beta_2 = i\psi_{II}^{(0)}(0) \]
\[ K \alpha_2 e^{-Kz} - K \beta_2 e^{Kz} + i\alpha_3' e^{iQz} = -i\psi_{II}^{(0)}(a) \] (3.26)

The solution of this system is

\[ \beta_1 = -\frac{i}{K} a_3 e^{iqz} \sinh aK - \frac{4q}{D} a_1 \sinh aK \]
\[ \alpha_2 = -ia_3 e^{iqz} \frac{e^{Kz}}{2K} = \frac{a_2}{q + iK} \]
\[ \beta_2 = i a_3 e^{iqz} \frac{e^{-Kz}}{2K} = \frac{b_2}{q - iK} \]
\[ \alpha_3' = 0 \] (3.27)

In the following, we consider \( Q/K = \gamma K/4 \gamma_c \) but also \( q/K \) as first order terms and we look for solutions up to the first order. The term in the reflected wave function arising from
$Q\beta_1$ is a second-order contribution which has to be neglected. Note that, in Region $I$, if the incident wave has the wave vector $q$, the reflected wave should have the wave vector $-q'$, where $q = q_0 - \delta q$ and $q' = q_0 + \delta q$. From Eq. [B27] it can be verified that $\delta q = (\gamma/4\gamma_c) q_0^2 = (q_0/K)^2 Q$. Then $\delta q$ is a second-order term which has to be neglected so that media $I$ and $III$ have no sizable spin splitting. This indicates that the solution we obtain in the case of a constant $\gamma$ also constitutes a plausible physical solution when $\gamma$ is a step function, with $\gamma = 0$ outside the barrier. Also note that, at this level of approximation, $\varphi^S$ is a wave which only exists inside the barrier and is not coupled to the free-electron waves outside the barrier. Because $A_3 = a_3 e^{iQa}$, we see that there is a pure dephasing between the up- ($Q_1 = Q$) and the down- ($Q_1 = -Q$) spin channels.

We have to be sure that, in our treatment, the probability current is conserved along the tunnel process. The wave in the barrier, in the up-spin channel, is of the form $\psi(z) = (A_2 e^{-Kz} + B_2 e^{Kz}) e^{iQz} = \phi(z) e^{iQz}$ with $A_2 = a_2 (1 - iQ/K)$ and $B_2 = b_2 (1 + iQ/K)$. Let us calculate $J$ to the first order in $Q$ by making use of Eq. 2.14

$$J[\psi] = J_+ [\psi] = J^f [\psi] + \frac{\gamma}{2\hbar} \left[ \frac{2}{2} \left| \frac{\partial \psi^{(0)}}{\partial z} \right|^2 - \psi^{(0)*} \frac{\partial^2}{\partial z^2} \psi^{(0)} - \psi^{(0)} \frac{\partial^2}{\partial z^2} \psi^{(0)*} \right]$$

(3.28)

It is sufficient to evaluate the term in the bracket to the zeroth order, substituting $\psi$ with $\psi^{(0)}$. One finds

$$J[\psi] = J^f [\psi] + \frac{\gamma}{2\hbar} \left[ \left. \frac{\partial \psi^{(0)}}{\partial z} \right|^2 - \psi^{(0)*} \frac{\partial^2}{\partial z^2} \psi^{(0)} - \psi^{(0)} \frac{\partial^2}{\partial z^2} \psi^{(0)*} \right]$$

$$\approx J^f [\psi] + 2 \frac{\gamma_c Q}{\hbar K} \left[ \left| \frac{\partial \psi^{(0)}}{\partial z} \right|^2 - 2K^2 \left| \psi^{(0)} \right|^2 \right]$$

(3.29)

$$= J^f [\psi] - 2 \frac{\gamma_c Q}{\hbar} \left[ \left| \psi^{(0)} \right|^2 + 2 (a_2 b_2 + a_2 b_2^*) \right]$$

with

$$J^f [\psi] = \text{Im} \left( \frac{\psi^{*} \hbar}{m} \frac{\partial \psi}{\partial z} \right) = \frac{2\gamma_c}{\hbar} \text{Im} \left( \frac{\phi^*}{\partial z} \right) + \frac{2\gamma_c Q}{\hbar} \left| \psi^{(0)} \right|^2$$

(3.30)

$$J^f [\psi] = \frac{2\gamma_c}{\hbar} \text{Im} \left( \frac{\psi^{(0)*} \partial \psi^{(0)}}{\partial z} \right) + \frac{4\gamma_c Q}{\hbar} (a_2 b_2 + a_2 b_2^*) + \frac{2\gamma_c Q}{\hbar} \left| \psi^{(0)} \right|^2$$

(3.31)

By comparing these expressions, one obtains

$$J[\psi] = \frac{2\gamma_c}{\hbar} \text{Im} \left( \frac{\psi^{(0)*} \partial \psi^{(0)}}{\partial z} \right) = J^f [\psi^{(0)}]$$

(3.32)
This definitely establishes current conservation in the tunnel process.

Starting with an incident state \( |\varphi_0\rangle \), the transmission asymmetry \( T \) in the spin-dependent tunneling process can be expressed as

\[
T = \frac{||T(|\varphi_0\rangle)||^2 - ||T(\hat{K}|\varphi_0\rangle)||^2}{||T(|\varphi_0\rangle)||^2 + ||T(\hat{K}|\varphi_0\rangle)||^2}
\]  

(3.33)

In the present case, we find \( T = 0 \). Whatever the incident spin, the tunnel barrier acts as a pure spin rotator, without any spin filter effect.

The cases of a spin-split quantum well confined between infinite walls and grown along the [110] direction is discussed in Appendix B2.

2. A unified description

Let us now consider transport in the real conduction band, in Region I or III. In the case \( \gamma = 0 \), the solution of the Schrödinger equation is

\[
\psi(z) = \psi^{(0)}(z) = a_j e^{iq_0 z} + b_j e^{-i q_0 z},
\]

\( j = 1 \) or \( 3, b_3 = 0 \). When \( \gamma \) is non zero, the wave function, in the up-spin channel, has to be of the form

\[
\psi(z) = e^{i \vartheta} \left[ a_j \left( 1 + \alpha \frac{\delta q}{q_0} \right) e^{i q_0 z} + b_j \left( 1 + \beta \frac{\delta q}{q_0} \right) e^{-i q_0 z} \right] e^{-i \delta q z}
\]

(3.34)

where \( e^{i \vartheta} \) is a phase factor. Here again, let us calculate \( J \) to the first order in \( \delta q \) by making use of Eq. (3.28). Substituting \( \psi \) with \( \psi^{(0)} \) in the bracket, one obtains

\[
J[\psi] \approx J^f[\psi] + \frac{\gamma}{2\hbar} \left[ \frac{\partial \psi^{(0)}}{\partial z} \right]^2 + 2 q_0^2 |\psi^{(0)}|^2 \right]
\]

\[
= J^f[\psi] + 2 \gamma \frac{c}{\hbar} \delta q \left[ 3 |\psi^{(0)}|^2 - 2 \left( a_j^* b_j e^{2i q_0 z} + a_j b_j^* e^{-2i q_0 z} \right) \right]
\]

(3.35)

\[
J^f[\psi] = J^f[\psi^{(0)}] + 4 \gamma \frac{c}{\hbar} \delta q \left( |a_j|^2 \text{ Re } \alpha - |b_j|^2 \text{ Re } \beta \right) - 2 \gamma \frac{c}{\hbar} \delta q |\psi^{(0)}|^2
\]

(3.36)

For \( \text{ Re } \alpha = -\text{ Re } \beta \), one finds

\[
J^f[\psi] = J^f[\psi^{(0)}] + 4 \gamma \frac{c}{\hbar} \delta q \text{ Re } \alpha \left( |a_j|^2 + |b_j|^2 \right) - 2 \gamma \frac{c}{\hbar} \delta q |\psi^{(0)}|^2
\]

(3.37)
Taking $\text{Re} \alpha = -1$ and $\text{Im} \alpha = \text{Im} \beta = 0$,

$$
\mathbf{J}[\psi] = \mathbf{J}^f[\psi^{(0)}] \quad (3.38)
$$

In the barrier, we consider (cf Sec. III B 1)

$$
\psi_B(z) = \left[ a_z \left( 1 - i \frac{Q}{K} \right) e^{-Kz} + b_z \left( 1 + i \frac{Q}{K} \right) e^{Kz} \right] e^{iQz} \quad (3.39)
$$

$$
\psi_B(z_0) e^{-iQz_0} = (a_z e^{-Kz_0} + b_z e^{Kz_0}) - i \frac{Q}{K} (a_z e^{-Kz_0} - b_z e^{Kz_0}) \quad (3.40)
$$

$$
\psi_B(z_0) = e^{iQz_0} \left[ \psi^{(0)}(z_0) + i \frac{Q}{K^2} \partial \psi_B^{(0)}(z_0) \right] = e^{iQz_0} \left[ \psi^{(0)}(z_0) + i \frac{\gamma_2}{4 \gamma_{2c}} \partial \psi_B^{(0)}(z_0) \right] \quad (3.41)
$$

In the well, let us take (cf Eq. 3.34)

$$
\psi_W(z) = e^{iQz_0} \left[ a_j \left( 1 - \frac{\delta q_j}{q_j0} \right) e^{iq_jaz} + b_j \left( 1 + \frac{\delta q_j}{q_j0} \right) e^{-iq_jaz} \right] e^{-i\delta q_j(z-z_0)} \quad (3.42)
$$

where $z_0$ is the boundary relevant to the region of the well (e.g. $z_0 = 0$ in Region I and $z_0 = a$ in Region III). Although we are still dealing with a unique effective mass and a constant $\gamma$, for the subsequent discussion, it is convenient to refer to $\gamma (\gamma_{c})$ as $\gamma_2 (\gamma_{2c})$ or $\gamma_j (\gamma_{jc})$ where $j = 1$ or 3 in the different regions, and to the wave vectors as $q_j0 - \delta q_j$ and $- (q_j0 + \delta q_j)$.

$$
\psi_W(z_0) = e^{iQz_0} \left[ \psi^{(0)}(z_0) + \frac{\delta q_j}{q_j0} \partial \psi_W^{(0)}(z_0) \right] = e^{iQz_0} \left[ \psi^{(0)}(z_0) + i \frac{\gamma_j}{4 \gamma_{jc}} \partial \psi_W^{(0)}(z_0) \right] \quad (3.44)
$$

We obtain

$$
\psi_B(z_0) - \psi_W(z_0) = e^{iQz_0} \left[ i \frac{\gamma_2}{4 \gamma_{2c}} \frac{\partial \psi_B^{(0)}(z_0)}{\partial z} - i \frac{\gamma_j}{4 \gamma_{jc}} \frac{\partial \psi_W^{(0)}(z_0)}{\partial z} \right]
$$

$$
= e^{iQz_0} \frac{i}{4 \gamma_{jc}} \frac{\partial \psi_B^{(0)}(z_0)}{\partial z} \left( \frac{\gamma_2 \gamma_{jc}}{\gamma_{2c}} - \frac{\gamma_j \gamma_{2c}}{\gamma_{jc}} \right)
$$

$$
= e^{iQz_0} \frac{i}{4 \gamma_{2c}} \frac{\partial \psi_W^{(0)}(z_0)}{\partial z} \left( \frac{\gamma_2 \gamma_{jc}}{\gamma_{2c}} - \frac{\gamma_j \gamma_{2c}}{\gamma_{jc}} \right) \quad (3.45)
$$

Here, we have used the relation

$$
\gamma_{2c} \frac{\partial \psi_B^{(0)}(z_0)}{\partial z} = \gamma_{jc} \frac{\partial \psi_W^{(0)}(z_0)}{\partial z} \quad (3.46)
$$
which originates from the usual relation expressing current conservation in the absence of DP field. When \( \gamma \) and \( \gamma_c \) (i.e. \( m \)) are constant, \( \psi_B(z_0) - \psi_W(z_0) = 0 \), which establishes the continuity of the wave function.

Now, let us examine the matching conditions of the derivative

\[
\psi_B(z) = \left[ a_2 \left( 1 - i \frac{Q}{K} \right) e^{-Kz} + b_2 \left( 1 + i \frac{Q}{K} \right) e^{Kz} \right] e^{iQz} \tag{3.47}
\]

\[
\frac{\partial \psi_B(z_0)}{\partial z} = e^{iQz_0} \left\{ \left[ -K a_2 \left( 1 - i \frac{Q}{K} \right) e^{-Kz_0} + K b_2 \left( 1 + i \frac{Q}{K} \right) e^{Kz_0} \right] + iQ \left( a_2 e^{-Kz_0} + b_2 e^{Kz_0} \right) \right\}
\]

\[
\frac{\partial \psi_W(z_0)}{\partial z} = e^{iQz_0} \left\{ iq_j \left[ a_j \left( 1 - \delta q_j \right) e^{iq_jz_0} - b_j \left( 1 + \delta q_j \right) e^{-iq_jz_0} \right] - i\delta q_j \psi(0)(z_0) \right\}
\]

\[
\gamma_{2c} \frac{\partial \psi_B(z_0)}{\partial z} - \gamma_{jc} \frac{\partial \psi_W(z_0)}{\partial z} = e^{iQz_0} \left\{ \left[ \gamma_{2c} \frac{\partial \psi_B^{(0)}(z_0)}{\partial z} - \gamma_{jc} \frac{\partial \psi_W^{(0)}(z_0)}{\partial z} \right] + 2i \left( \gamma_{2c} Q + \gamma_{jc} \delta q_j \right) \psi(0)(z_0) \right\}
\]

\[
= \frac{1}{2i} \left( \gamma_{2c} K^2 + \gamma_{jc} q_j^2 \right) e^{iQz_0} \psi(0)(z_0) \tag{3.50}
\]

This is exactly the jump of the derivative calculated in Eq. 3.14 up to the second-order terms. Thus, starting from the standard solution, we have constructed in a very simple way a wave function which is continuous, associated to the constant current of probability \( J^f \left[ \psi^{(0)} \right] \), and which is the solution to the tunneling problem.

3. Insight into the step-function case

The case where \( \gamma(z) = \gamma_g(z) \) is not a constant raises difficult questions. The problem is not to solve Eqs. 3.16 but to define a proper Hamiltonian, which has to be Hermitian: This
would not be the case simply by substituting $\gamma$ with $\gamma(z)$ in these equations and there are several ways to symmetrize this Hamiltonian. This is in line with the BDD approach when dealing with an heterostructure where $m = m(z)$, i.e. where $m$ depends on $z$, for instance $m = m_1$ in Region $I$ and $m = m_2$ in Region $II$. In that case, the starting point is the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m(z)} \frac{\partial^2}{\partial z^2} + V \tag{3.51}$$

The key idea is to transform this equation by defining the BDD Hamiltonian

$$\hat{H}_{BDD} = \frac{\hbar}{2i} \frac{\partial}{\partial z} \hat{v} + V \tag{3.52}$$

where $\hat{v}$ is defined in Eq. 2.5. Then, an integration of the Schrödinger equation around the origin, exactly as performed above, will allow us to show that $J = \psi^* \hat{v} \psi$ is continuous because $\psi$ and $\frac{1}{m(z)} \frac{\partial \psi}{\partial z}$ are continuous. The BDD Hamiltonian guarantees probability-current conservation and the problem receives sound foundations. Unfortunately, the more complicated form of the current of probability given in Eq. 2.14 - in particular due to the $\left| \frac{\partial \psi}{\partial z} \right|^2$ term - makes an analogous transformation not obvious so that the general case still remains an open question. However, let us point out that, when the masses and the DP-field coefficients are not very different over the three regions - a frequent situation in heterostructures - through the procedure described in the preceding subsection, we are able to construct a wave which is continuous at the boundaries and that conserves the current of probability. Therefore, this wave is a plausible solution. The principle is first to solve the envelope-function problem in the absence of DP field, i.e. $g(z) = 0$, taking into account the mass discontinuities in framework of the BDD formalism. This determines the standard function $\psi^{(0)}(z)$. Secondly, the wave functions in the different regions are modified according to the rules defined in the preceding subsection (Eqs. 3.39 and 3.42). The current of probability remains equal to $J^I \left[ \psi^{(0)} \right]$ in the three regions. Concerning the continuity of the wave function at the boundaries, we have at $z_0 = 0$

$$\frac{\partial \psi^{(0)}_W (0)}{\partial z} \approx 2i q_1 a_1$$

$$\delta q \approx \frac{\gamma_1 \gamma_2 c}{\gamma_2 \gamma_1 c} q_1^2$$

and

$$Q \approx \frac{\gamma_2 c}{4 \gamma_2 c} K^2 \tag{3.53}$$

Thus (see Eq. 3.35)

$$\psi_B (0) - \psi_W (0) = -\frac{1}{2} q_1 a_1 \left( \frac{\gamma_2 c}{\gamma_2 c} - \frac{\gamma_2 c}{\gamma_j c} \right) \tag{3.54}$$
We introduce
\[ \gamma_{j,2} = \gamma_j + \gamma_2 \quad \text{and} \quad \delta \gamma_{j,2} = \frac{\gamma_j - \gamma_2}{2} \]
\[ \gamma_j = \gamma_{j,2} + \delta \gamma_{j,2} \quad \gamma_2 = \gamma_{j,2} - \delta \gamma_{j,2} \] (3.55)

\[ \Gamma_{j,2} = \frac{\gamma_{jc} + \gamma_{2c}}{2} \quad \text{and} \quad \delta \Gamma_{j,2} = \frac{\gamma_{jc} - \gamma_{2c}}{2} \]
\[ \gamma_{jc} = \Gamma_{j,2} + \delta \Gamma_{j,2} \quad \gamma_{2c} = \Gamma_{j,2} - \delta \Gamma_{j,2} \] (3.56)

\[ \psi_B(0) - \psi_W(0) = \frac{-1}{2} q_1 a_1 \gamma_{1,2} \left[ \left( 1 - \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} \right) \left( 1 + \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \right) - \left( 1 + \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} \right) \left( 1 - \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \right) \right] \]
\[ = \frac{q_1 a_1}{\gamma_{2c}} \gamma_{1,2} \left( \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} - 2 \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \right) \approx \frac{q_1 a_1}{\gamma_{2c}} \gamma_{1,2} \left( \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} - 2 \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \right) = 4 a_1 \frac{q_1 Q}{K} \left( \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} - 2 \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \right) \] (3.57)

At \( z_0 = a \), the situation is similar with
\[ \frac{\partial \psi_W^{(0)}(a)}{\partial z} = iq_3 a_3 e^{iQa} e^{iQa} \] (3.58)

In the case where \( \frac{\delta \gamma_{1,2}}{\gamma_{1,2}} \) and \( \frac{\delta \Gamma_{1,2}}{\Gamma_{1,2}} \) are small and considered as first-order terms, the discontinuities are third-order terms which can be safely neglected.

4. Quasi-classical picture (Regions I and III without sizable spin splitting)

In the case where Regions I and III have no sizable spin splitting, we develop a quasi-classical picture of the tunneling process. For an up spin \( Q = Q_\uparrow \), so that the wave function in the barrier writes as

\[ \psi_{II}(z) = \left[ a_2 \left( 1 - \frac{iQ}{K} \right) e^{-Kz} + b_2 \left( 1 + \frac{iQ}{K} \right) e^{Kz} \right] e^{iQz} \]
\[ = \psi_{II}^{(0)}(z) e^{iQz} + \left( \frac{iQ}{K} \frac{1}{K} \frac{1}{K} \frac{\partial}{\partial z} \psi_{II}^{(0)}(z) \right) e^{iQz} \] (3.59)

The wave function for the down spin is obtained by replacing \( Q \) by \( -Q \). We can combine the two spin channels to build the quasi-classical solution \( \psi^c(z) \) corresponding to an incident wave with a spin lying in the plane perpendicular to the DP field

\[ \psi_I^c(z) = (\lambda \uparrow + \lambda^* \downarrow) \psi_I^{(0)}(z) = S \lambda(0) \psi_I^{(0)}(z) \] (3.60)
which yields
\[
\psi_{II}^c(z) = \psi_{II}^{(0)}(z)S_\lambda(z) - \frac{Q}{K} \frac{1}{K} \frac{\partial}{\partial z} \psi_{II}^{(0)}(z) i \hat{K} S_\lambda(z)
\]  
(3.61)

Defining
\[
\tan \theta = \frac{Q}{K} \approx \theta
\]  
(3.62)

we can write to the first order
\[
\psi_{II}^c(z) = \cos \theta \psi_{II}^{(0)}(z)S_\lambda(z) - \sin \theta \frac{1}{K} \frac{\partial}{\partial z} \psi_{II}^{(0)}(z) i \hat{K} S_\lambda(z)
\]  
(3.63)

The transmitted wave is
\[
\psi_{III}^c = \left( \lambda e^{iQa} \uparrow + \lambda^* e^{-iQa} \downarrow \right) a_3 e^{iqz} = S_\lambda(a) \psi_{III}^{(0)}
\]  
(3.64)

The incident wave corresponds to a spin lying in the \( \Pi \chi \) plane, normal to \( \chi(\mathbf{e}_{110}) \). An important result is that the transmitted wave has the spin \( S_\lambda(a) \), i.e. rotated by the angle \(-2Qa\). We can estimate the angle \( 2Qa \approx 0.2 \left( K/1 \, \text{Å}^{-1} \right)^2 (a/1 \, \text{Å}) \) in GaAs along the [110] direction, the largest reasonable value of \( K \) being smaller than 0.1 \( \text{Å}^{-1} \), a value beyond which the spin-splitting in \( k^3 \) is no longer valid. The spin-split barrier appears to exert a spin torque which produces a rotation of the spin of the transmitted electron around the quantization axis, which is the direction of the DP field. There is no spin transmission asymmetry. The spin-orbit-split barrier acts as a spin rotator inside the \( \Pi \chi \) plane. This has some analogy with the reflection of a neutron beam on a ferromagnetic mirror discussed in Ref. 28 which physically results from spin precession during the time spent by the evanescent wave inside the barrier. But, in this example, this straightforwardly arises from the difference in the reflection and transmission coefficients for the two spin eigenstates.

Anyway, this spin precession provides an estimation of the tunnel time \( \tau \), by using this built-in Larmor clock\( ^{29} \) The effective field is determined through: \( \hbar \Omega \approx 2\gamma |\chi| \) whereas \( \Omega \tau = 2Qa \approx |a\gamma \chi_e/\gamma_c| K^2 \). We find \( \tau \approx |a\hbar/2\gamma| |\chi_e/\chi| K^2 \). In the [110] direction, \( \chi_e = 1/2 \) (see Sec. IIIB) so that \( \tau \approx |a\hbar/4\gamma_c K| \approx 10^{-18} (a/1 \, \text{Å}) \left( 1 \, \text{Å}^{-1}/K \right) \) s.

We recognize that the in-plane solution belongs to the subspace of free-electron-current conserving waves studied in Sec. IIIC4. In that sense, we have restored a ”classical” tunneling process. Note that \( \mathbf{J} = \mathbf{J}^f \) is a constant, but the classical ”magnetic current” in Region II, \( \delta \mathbf{J}^f(z) = \mathbf{J}^f_\uparrow(z) - \mathbf{J}^f_\downarrow(z) \) is not and undergoes a discontinuity at the boundaries. Quite generally for any two-component spinor \( \psi = \psi_\uparrow \uparrow + \psi_\downarrow \downarrow \) with \( \psi_\uparrow = \Phi e^{iQz} \) and
\[\psi_0 = \Phi e^{-iQz}\]

\[
\begin{align*}
\mathbf{J}_f[\psi_\pm] &= \frac{\hbar}{m} \text{Im} \left[ \psi_\mp^* \nabla \psi_\pm \right] \\
\delta \mathbf{J}_f &= \mathbf{J}_f[\psi_+] - \mathbf{J}_f[\psi_-] = \frac{\hbar}{m} \text{Im} \left[ \psi_+^* \nabla \psi_+ - \psi_-^* \nabla \psi_- \right] \\
\delta \mathbf{J}_f &= \frac{\hbar}{m} \text{Im} \left[ (\psi_+ \uparrow - \psi_- \downarrow) \nabla (\psi_+ \uparrow + \psi_- \downarrow) \right] = \frac{1}{m} \text{Re} \left[ \psi_+^* (\hat{\mathbf{p}} \cdot \hat{\mathbf{\sigma}}) \psi \right]
\end{align*}
\] (3.65a)

Thus, the jump of \(\delta \mathbf{J}_f\) is

\[
[\delta \mathbf{J}_f]_{z_0}^0 = \frac{\hbar}{m} \text{Im} \left\{ (\hat{\sigma}_z \psi)_z^0 \nabla \psi]_{z_0}^0 \right\} = \frac{1}{m} \text{Re} \left[ \psi_+^* (\hat{\mathbf{p}} \cdot \hat{\mathbf{\sigma}}) \psi \right]_{z_0}^0
\] (3.66)

More explicitly, we have \(\delta \mathbf{J}_f = \delta \mathbf{J}_{III} = 0\), \(\delta \mathbf{J}_{II}(z) \simeq 2 |\lambda|^2 \frac{\hbar Q}{m} \frac{1}{K} \frac{\partial \Phi_{II}(z)}{\partial z}\). This can be viewed as a kinetic-momentum transfer along the internal-field direction during the tunnel process, in strong analogy with the spin transfer resulting from spin torque in ferromagnetic structures, as introduced by Slonczewski and Berger.9,10

**IV. ORTHO PROCESS: [001]-ORIENTED BARRIER UNDER ALMOST NORMAL INCIDENCE**

It is not possible to stay in simple band schemes - like in Fig. 3 - as \(\xi\) has to be conserved: The relevant scheme is drawn in Fig. 6. To simplify without altering the physics of interest, the component of the wave vector normal to [001] is taken parallel to [100]. The spin is quantized along the \(Oz\) axis, taken parallel to [001]. As shown below, the eigenstates of the spin are in a direction normal to \(Oz\). The energy writes

\[
E = -\gamma_c (K^2 - \xi^2) \pm \gamma \xi K \sqrt{K^2 - \xi^2}
\] (4.1)

\[
(E + \gamma_c (K^2 - \xi^2)) = (\gamma \xi K)^2 (K^2 - \xi^2)
\] (4.2)

where the generic wave vector is \(\xi \mathbf{e}_{100} + iK \mathbf{e}_{001}\). This equation may admit 4 real roots, \(\pm K\), and \(\pm K'\). The states of the four wave vectors \((\xi, 0, iK) \uparrow_k, (\xi, 0, -iK) \uparrow_{k'}, (\xi, 0, iK) \downarrow_{k'}, (\xi, 0, -iK) \downarrow_{k'}\) have the same energies: \(K\) and \(K'\) are such that \(E \uparrow (K) = E \downarrow (K')\). Note that Kramers conjugate states, which would involve \(-\xi\), are not relevant because \(\xi\) is conserved. We introduce \(K_0 = (K' + K)/2\) and \(\delta K = K' - K\) (note that this definition differs by a factor of 2 of the definition used in Sec. III, where \(2\delta q = q' - q\); The choice made in the present section makes more easy the comparison with the results derived in Ref. 13).
We assume that $K' > K > 0$ so that $\delta K > 0$. Moreover, as in Ref. 13, the incident-wave energy is smaller than half of the barrier energy, which means that $q < K$.

As recognized by Perel’ et al., the tunneling problem admits simple $C^1$ solutions under the approximation $\xi/K_0 \ll 1$. Besides, the spin asymmetry which originates from the spin-orbit interaction is characterized by the ratio $\delta K/K_0$, which, from band-structure calculations and from spin-precession experiments, is known to be small, i.e. $\delta K/K_0 \ll 1$. We further assume that $aK_0$ is not small compared to unity, which corresponds to a barrier of small transparency, and consequently we have $\exp(-2aK_0) \ll 1$. These three quantities, $\xi/K_0$, $\delta K/K_0$, and $\exp(-2aK_0)$ will be hereafter taken as first-order quantities and we will look for solutions to the first order only. This does not imply that the quantity $a\delta K = (aK_0)(\delta K/K_0)$, which is of crucial interest as it characterizes the spin selectivity of the barrier (as illustrated by the simple evaluation indicated below), is smaller than unity. In the physical problem, we consider electron tunneling under off-normal incidence and the angle of incidence is significant only when $q$ and $\xi$ are of the same order, which means $q/K_0 \ll 1$. We shall use this additional approximation only when it will be necessary to get analytical expressions of the wave vectors (Subsec. IV C). Intuitively, if we start with an unpolarized electron beam, the up- (down-) spin electrons merge from the barrier with an amplitude of probability almost proportional to $\exp(-aK)$ (respectively $\exp(-aK')$) so that the current asymmetry - which, in this case, is also the polarization $\Pi$ of the current - is given by

$$\Pi \approx \frac{e^{-2aK} - e^{-2aK'}}{e^{-2aK} + e^{-2aK'}} = \tanh a\delta K \quad (4.3)$$

Indeed, in Ref. 13, it is found that the polarization $P$ of the transmitted current, when the primary beam is not polarized, is $P \approx \tanh a\delta K$ (see below Eq. 4.15). In practical cases, $a\delta K$ cannot be larger than a (often small) fraction of unity. Nevertheless, in the calculation, we do not put any restrictive assumption on $a\delta K$ (which is not assumed to be a first-order quantity) and we will calculate eigenvectors, when required, as a power expansion in $a\delta K$, but, obviously, we keep in mind that the first-order term will generally be sufficient to reach a reasonable accuracy.
A. Zeroth-order wave functions

The wave vectors $K$ and $K'$ are related through the equation ($K' > K$ and assuming $\gamma > 0$ for the sake of simplicity)

$$-\gamma_c(K^2 - \xi^2) - \gamma\xi K\sqrt{K^2 - \xi^2} = -\gamma_c(K'^2 - \xi^2) + \gamma\xi K'\sqrt{K'^2 - \xi^2}$$  \hspace{1cm} (4.4)

or

$$\gamma_c(K'^2 - K^2) = \gamma\xi \left( K\sqrt{K^2 - \xi^2} + K'\sqrt{K'^2 - \xi^2} \right)$$  \hspace{1cm} (4.5)

Up to the first order in $\delta K/K_0$, Eq. 4.5 writes as

$$2\gamma_c K_0\delta K = 2\gamma\xi K_0\sqrt{(K_0^2 - \xi^2)}$$  \hspace{1cm} (4.6)

or

$$\delta K = \frac{\gamma\xi K_0}{\gamma_c} \sqrt{1 - \frac{\xi^2}{K_0^2}} \approx \frac{\gamma\xi K_0}{\gamma_c}$$  \hspace{1cm} (4.7)

We now calculate the eigenvectors. Let us write $k = (\xi, 0, \eta i K)$ with $\eta = \pm 1$, $\mathcal{K} = K$ or $K'$, $\xi$, $K$ and $K' > 0$. $\chi = \mathcal{K}\xi(K, 0, i\eta\xi)$.

The eigenvalues of $\hat{\sigma} \cdot \chi = \begin{bmatrix} \chi_z & \chi_x - i\chi_y \\ \chi_x + i\chi_y & -\chi_z \end{bmatrix}$ are $\pm\xi\mathcal{K}\sqrt{\mathcal{K}^2 - \xi^2}$.

To the first order in $\xi/K_0$, the normalized eigenvectors $c_1 \uparrow + c_2 \downarrow = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$ are such that

wave vector

$$\begin{bmatrix} \xi \\ 0 \\ iK \end{bmatrix} \begin{bmatrix} \xi \\ 0 \\ -iK \end{bmatrix} \begin{bmatrix} \xi \\ iK \end{bmatrix} \begin{bmatrix} \xi \\ iK' \end{bmatrix} \begin{bmatrix} \xi \\ -iK' \end{bmatrix}$$  \hspace{1cm} (4.8)

spin $\times \sqrt{2}$

$$\begin{bmatrix} 1 + \frac{i\xi}{2K} \\ 1 - \frac{i\xi}{2K} \end{bmatrix} \begin{bmatrix} 1 - \frac{i\xi}{2K} \\ 1 + \frac{i\xi}{2K} \end{bmatrix} \begin{bmatrix} 1 - \frac{i\xi}{2K'} \\ 1 + \frac{i\xi}{2K'} \end{bmatrix} \begin{bmatrix} 1 + \frac{i\xi}{2K'} \\ 1 - \frac{i\xi}{2K'} \end{bmatrix}$$

Observe that $\uparrow_k$ and $\downarrow_k$ are not orthogonal (even in a first-order calculation - compare the first term to the third one after substituting $K'$ with $K$). Inside the barrier the wave
function is of the shape \( \Psi^{II}(r) = e^{i\xi \rho} \Psi^{II}(z) \) and

\[
\Psi^{II}(z) = A_2 \left[ \begin{array}{c}
1 + \frac{i\xi}{2K} \\
1 - \frac{i\xi}{2K}
\end{array} \right] e^{-Kz} + B_2 \left[ \begin{array}{c}
1 - \frac{i\xi}{2K} \\
1 + \frac{i\xi}{2K}
\end{array} \right] e^{Kz}
\]

\[
+ \tilde{A}_2 \left[ \begin{array}{c}
1 - \frac{i\xi}{2K'} \\
-(1 + \frac{i\xi}{2K'})
\end{array} \right] e^{-K'z} + \tilde{B}_2 \left[ \begin{array}{c}
1 + \frac{i\xi}{2K'} \\
-(1 - \frac{i\xi}{2K'})
\end{array} \right] e^{K'z}
\]

\[
= \left[ A_2 e^{-Kz} + B_2 e^{Kz} + \frac{i\xi}{2K'} \left( -\tilde{A}_2 e^{-K'z} + \tilde{B}_2 e^{K'z} \right) \right] \left[ \begin{array}{c}
1 \\
1
\end{array} \right]
\]

\[
+ \left[ \frac{i\xi}{2K} \left( A_2 e^{-Kz} - B_2 e^{Kz} \right) + \tilde{A}_2 e^{-K'z} + \tilde{B}_2 e^{K'z} \right] \left[ \begin{array}{c}
1 \\
-1
\end{array} \right]
\]  

(4.9)

Outside the barrier, we are looking for the solution of the shape:

\[
\Psi^{I}(z) = A_1 \left[ \begin{array}{c}
1 \\
1
\end{array} \right] e^{iqz} + B_1 \left[ \begin{array}{c}
1 \\
1
\end{array} \right] e^{-iqz} + \tilde{A}_1 \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] e^{iqz} + \tilde{B}_1 \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] e^{-iqz}
\]  

(4.10)

and

\[
\Psi^{III}(z) = A_3 \left[ \begin{array}{c}
1 \\
1
\end{array} \right] e^{iqz} + \tilde{A}_3 \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] e^{iqz}
\]  

(4.11)

The wave function writes as

\[
\Psi^{I}(z) = \left[ A_1 e^{iqz} + B_1 e^{-iqz} \right] \left[ \begin{array}{c}
1 \\
1
\end{array} \right] + \left[ \tilde{A}_1 e^{iqz} + \tilde{B}_1 e^{-iqz} \right] \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] \]  

(4.12a)

\[
\Psi^{II}(z) = \left[ A_2 e^{-Kz} + B_2 e^{Kz} + \frac{i\xi}{2K'} \left( -\tilde{A}_2 e^{-K'z} + \tilde{B}_2 e^{K'z} \right) \right] \left[ \begin{array}{c}
1 \\
1
\end{array} \right] \]

\[
+ \left[ \frac{i\xi}{2K} \left( A_2 e^{-Kz} - B_2 e^{Kz} \right) + \tilde{A}_2 e^{-K'z} + \tilde{B}_2 e^{K'z} \right] \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] \]  

(4.12b)

\[
\Psi^{III}(z) = \left[ A_3 e^{iqz} \right] \left[ \begin{array}{c}
1 \\
1
\end{array} \right] + \left[ \tilde{A}_3 e^{iqz} \right] \left[ \begin{array}{c}
1 \\
-1
\end{array} \right] \]  

(4.12c)

The continuity of the wave function (Eqs. (4.12)) and of its derivative at \( z = 0 \) and \( z = a \) provides a linear system of 8 equations. A full discussion is given in Appendix C. This calculation has strong similarities with Slonczewski’s approach of the tunneling between two ferromagnets separated by a barrier, because we deal with two coupled spin channels.
B. Polarization

The transmission asymmetry $T$ is

$$ T = \frac{|t^+|^2 - |t^-|^2}{|t^+|^2 + |t^-|^2} $$

(4.13)

with $|t^+|^2 = |A_3^+|^2$ (calculated when $A_1 = 1$, $\bar{A}_1 = 0$) and $|t^-|^2 = |\tilde{A}_3^-|^2$ (calculated when $A_1 = 0$, $\bar{A}_1 = 1$). All the coefficients $A_j$ and $\tilde{A}_j$ are calculated in Appendix C.

To the zeroth order in $\xi/K_0$, $t^\pm = t^\pm_0$, $T = T_0$. Now

$$ |t^+_0|^2 = \frac{4qKe^{-Ka_0}}{(K - iq)^2} \quad ; \quad |t^-_0|^2 = \frac{4qK' e^{-K'a_0}}{(K' - iq)^2} $$

(4.14)

and we get the result of Ref. 13 namely

$$ T_0 = \tanh a \delta K $$

(4.15)

Up to the first order in $\xi/K_0$, $t^\pm = t^\pm_1$, $T = T_1$, $|t^+_1|^2 = \left( |A_3^+|^2 + |\tilde{A}_3^-|^2 \right)$ but $|\tilde{A}_3^+|^2$ and $|A_3^-|^2$ are of second order in $\xi/K_0$ so that, up to the first order in $\xi/K_0$, the result is the same as for the zeroth order: $T_0 = T_1$.

It is easy to show that this transmission asymmetry is nothing but the spin polarization of the transmitted beam when the primary beam is unpolarized, $T_0 = T_1 = \mathcal{P}$. As we have only assumed that $q < K_0$, we may wonder why the ratio $q/K_0$ does not appear in $\mathcal{P}$. The answer is given if we perform the calculation one order further in $\delta K/K_0 \ll 1$. Then, a lengthy calculation leads to

$$ \mathcal{P} = \frac{\tanh a \delta K + \frac{K_0 - q \delta K}{K_0 + q} \frac{\delta K}{K_0} \tanh a \delta K}{1 + \frac{K_0 - q \delta K}{K_0 + q} \frac{\delta K}{K_0} \tanh a \delta K} $$

(4.16)

In the limit where $\delta K/K_0$ is negligible, $\mathcal{P} = \tanh a \delta K$ is recovered.

Let us consider the transmission of a primary electron beam with an initial current polarization $P_i$ through a spin-filtering structure characterized by the transmission coefficients $e^{-2aK'}$ ($e^{-2aK}$) for up (down) - spin electrons. As the incident up- (down-) spin current is proportional to $1 + \mathcal{P}_i$ (respectively $1 - \mathcal{P}_i$), the current polarization of the emerging beam is simply given by $\mathcal{P}$

$$ \mathcal{P} = \frac{(1 + \mathcal{P}_i) e^{-2aK} - (1 - \mathcal{P}_i) e^{-2aK'}}{(1 + \mathcal{P}_i) e^{-2aK} + (1 - \mathcal{P}_i) e^{-2aK'}} = \frac{\mathcal{P}_i + \Pi}{1 + \Pi \mathcal{P}_i} $$

(4.17)
where \( \Pi \) is given by Eq. 4.3. The above formula yielding the polarization of the transmitted beam is a standard expression for spin filters (in spin polarimetry, \( \Pi \) is referred to as the Sherman function). Thus, \( \mathcal{P} \) in Eq. 4.43 appears to result from the combination of a primary-electron-beam polarization \( \mathcal{P}_i \approx -\delta K/K_0 \) when \( q/K_0 \ll 1 \), which does not depend on the barrier thickness, with the spin asymmetry of the material, \( \Pi = \tanh(a \delta K) \). The initial polarization \(-\delta K/K_0\) could be straightforwardly understood as resulting from the band mismatch, an interface effect. If this analogy provides us with a useful physical insight, it must, however, be realized that the above calculation is only valid when \( \exp aK_0 \gg 1 \) and cannot be extrapolated to \( a = 0 \). In any case, it is clear that \( P_i \) builds up in the early stage of the transport process.

### C. \( \xi/K_0 \) first-order wave function

It is shown in Appendix C that there is no \( \xi/K_0 \) first-order term in \( A_2, A_3, B_1, \) and \( B_2 \). We are therefore going to calculate \( \xi/K_0 \) first-order terms in \( \tilde{A}_2, \tilde{A}_3, \tilde{B}_2, \) and \( \tilde{A}_3 \). To be consistent with Subsec. IV A, we assume that \( A_1 \neq 0 \) and \( \tilde{A}_1 = 0 \). We obviously have to invert the role of \( K \) and \( K' \) if we start from \( A_1 = 0 \) and \( \tilde{A}_1 \neq 0 \). Let us recall that the calculation is performed with \( \delta K/K_0 \ll 1 \) which is always true and \( \xi/K_0 \ll 1 \).

Eqs. C1e, C1f, C1g, C1h give

\[
\begin{align*}
-\tilde{A}_2 \left( 1 - \frac{iq}{K'} \right) + \tilde{B}_2 \left( 1 + \frac{iq}{K'} \right) &= \frac{i\xi}{2K'} \left( 1 - \frac{iq}{K} \right) A_2 + \frac{i\xi}{2K'} \left( 1 + \frac{iq}{K} \right) B_2 \\
-\tilde{A}_2 \left( 1 + \frac{iq}{K'} \right) e^{-K'a} + \tilde{B}_2 \left( 1 - \frac{iq}{K'} \right) e^{K'a} &= \frac{i\xi}{2K'} \left( 1 + \frac{iq}{K} \right) A_2 e^{-K'a} + \frac{i\xi}{2K'} \left( 1 - \frac{iq}{K} \right) B_2 e^{K'a}
\end{align*}
\]

\(4.18a\)

\(4.18b\)

The determinant of the system defined by Eqs. 4.18 is

\[
\text{Det} = \left( 1 + \frac{iq}{K'} \right)^2 e^{-K'a} - \left( 1 - \frac{iq}{K'} \right)^2 e^{K'a}
\]

\(4.19\)

which differs from zero, therefore \( \tilde{A}_2 \) and \( \tilde{B}_2 \) can be calculated. We assume \( a \neq 0 \) (the case \( a = 0 \) has no interest) and we obtain

\[
\tilde{A}_2 = -\frac{i\xi}{2K'} \left[ A_2 e^{a\delta K/2} \frac{\sinh(K_0a)}{\sinh(K'a)} + B_2 e^{K_0a} \frac{\sinh(a\delta K/2)}{\sinh(K'a)} \right]
\]

\(4.20\)
and

\[
\tilde{B}_2 = \frac{i\xi}{2K'} \left[ A_2 e^{-K_0a} \frac{\sinh (a \delta K / 2)}{\sinh (K' a)} + B_2 e^{-a \delta K / 2} \frac{\sinh (K_0 a)}{\sinh (K' a)} \right] \quad (4.21)
\]

Noticing that i) \(\xi/K' = \xi/K_0 (1 + \delta K / 2K) \approx (\xi/K_0) (1 - \delta K / 2K_0) \approx \xi/K_0\) (the same result holds for \(\xi/K \approx \xi/K_0\)), ii) \(a \delta K < a K\), iii) \(A_2 \propto A_1\) (Eq. ??), and iv) \(B_2 \propto A_1 \exp (-2K a)\) (Eq. ??), we get

\[
\tilde{A}_2 \approx -\frac{i\xi}{2K_0} A_2 e^{-a \delta K / 2} \frac{\sinh (K_0 a)}{\sinh (K' a)}
\quad (4.22a)
\]

\[
\tilde{B}_2 = \frac{i\xi}{2K_0} \left[ A_2 e^{-K_0a} \frac{\sinh (a \delta K / 2)}{\sinh (K' a)} + B_2 e^{-a \delta K / 2} \frac{\sinh (K_0 a)}{\sinh (K' a)} \right]
\quad (4.22b)
\]

From now on we assume that \(\exp K_0 a \gg 1\) so that \(\sinh K_0 a / \sinh K' a = \exp -a \delta K / 2\) and

\[
\tilde{A}_2 \approx -\frac{i\xi}{2K_0} A_2 \quad (4.23)
\]

A lengthy calculation shows that:

i) \(\tilde{B}_1\) is proportional to \((\xi/K_0) (\delta K / K_0)\) and therefore is negligible. However, we can note that \(\tilde{B}_1\) is not strictly equal to zero so that the reflected wave has a \([1-1]^t\) component even though the incident wave has only a \([1 1]^t\) component.

ii)

\[
\tilde{B}_2 \approx \frac{i\xi}{2K_0} e^{-a \delta K} \left[ 2 \frac{iK + q}{iK - q} e^{-a \delta K / 2} \sinh \frac{a \delta K}{2} + 1 \right] B_2
\quad (4.24)
\]

We furthermore assume that \(q/K_0 \ll 1\) so that

\[
\tilde{B}_2 \approx \frac{i\xi}{2K_0} e^{-a \delta K} \left[ 2 - e^{-a \delta K} \right] B_2
\quad (4.25)
\]

and eventually

\[
\tilde{A}_3 = \frac{i\xi}{2K_0} \left( \sinh \frac{a \delta K}{2} - 2 \sinh^2 \frac{a \delta K}{2} \right) A_3
\quad (4.26)
\]

There is no assumption on \(a \delta K\) in Eq. ??.

We note that, as \(\tilde{A}_3\) differs from zero, the incident wave with only a \([1 1]^t\) spin component is transmitted with a component along the \([1 - 1]^t\) spin direction. This means there is not a pure spin-filter effect along the \(x\)-quantization axis.\textsuperscript{34}

V. CONCLUSION

Electron tunneling in a semiconductor with no inversion symmetry and in the presence of spin-orbit coupling involves complex wave vectors in the barrier. In directions where the
D’yakonov-Perel’ (DP) field is non zero, the problem becomes highly non-trivial. We have distinguished two particular types of tunnel processes: Para-type process where we have one-dimensional tunneling with a complex wave vector and ortho-type process associated with a complex wave vector with orthogonal real and imaginary components. For a para-process, the DP field is a complex vector but it remains collinear to a real direction so that the eigenvectors are orthogonal spin states. We have shown that, along the [110] direction no $C^1$ solution exists. The expression of the current of probability is re-examined, proper boundary conditions are derived, and a treatment of heterostructures is proposed. Quasi-classical states are shown to be in-plane solutions, which imply a pure spin rotation of the transmitted beam around the direction of the DP field. In the [110] direction, there is no spin-filter effect. This contrasts with the situation in the real conduction band where the spin-splitting is maximum along [110]. For an ortho-process, the DP field is a complex vector, which is not collinear to any real direction, and the eigenvectors of the Hamiltonian are no longer orthogonal spin states. Moreover, the evanescent eigenvectors are not associated with the same spin depending whether they propagate from left to right or from right to left. In this case, we have derived a first-order solution to the tunnel problem, which has strong similarities with standard off-normal tunneling, and an almost pure spin-filter effect was demonstrated, a conclusion consistent with the result of Perel’ et al.\textsuperscript{13} whose expression for the transmitted polarization has been corrected by the introduction of an initial interface polarization.

All these questions should now be addressed experimentally and we think that experiments are within reach. For instance, further developments of the study of the polarization of a reflected spin-polarized electron beam can be considered, in line with the measurements reported in Ref. 35. Polarized-luminescence experiments in quantum wells grown along the [110] axis could also bring valuable information, as well as measurements on resonant-tunneling devices or photogavalnic-effect measurements in coupled quantum wells.\textsuperscript{36,37,38,39} The results derived in the present article provide new insight in spin-dependent tunneling in solids whereas they also open stimulating perspectives for spin manipulation in tunnel devices.
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To solve such a problem, we only have to find usual formal solutions dealing with plane waves of vectors $\pm q$ outside the barrier and $\pm iK$ in the barrier respectively. This provides us with the reflection and transmission coefficients. Then, we obtain the true wave functions by multiplying the formal solutions by $e^{i\zeta \cdot r}$.

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APPENDIX A: EVANESCENT BAND IN THE [110] DIRECTION

Let us write $\mathbf{k} = (Q + iK)\mathbf{e}$, having in mind $\mathbf{e}$ along the [110] direction: $\mathbf{e} = e_{110} = \frac{1}{\sqrt{2}}[110]$. We have to find the relation between $Q$ and $K$ to get a real eigenvalue of the Hamiltonian $\hat{H}$. This real eigenvalue is the energy. The Hamiltonian $\hat{H}$ writes as

$$\hat{H} = \gamma_e (Q + iK)^2 + \gamma \hat{\sigma} \cdot \mathbf{\chi} = \gamma_e (Q + iK)^2 + \gamma \chi_e (Q + iK)^3 \hat{\sigma} \cdot \mathbf{e}_\chi$$

(A1)

$$\mathbf{e}_\chi = \chi / ||\chi|| \quad \text{(provided} \quad ||\chi|| \neq 0) \quad \mathbf{\chi} , \text{a dimensionless parameter, depends on the direction. If} \quad \mathbf{e} = e_{110}, \quad \chi \text{is parallel to} \quad e_{110} \text{with} \chi_e = 1/2. \quad \text{The eigenvalues are}$$

$$\mathbf{E}(\mathbf{k}) = \gamma_e (Q + iK)^2 + \epsilon \chi_e \gamma (Q + iK)^3$$

(A2)

The spin is quantized along $\gamma \mathbf{e}_\chi$ so that $\epsilon \gamma > 0$ corresponds to the spin $\uparrow$ and $\epsilon \gamma < 0$ corresponds to the spin $\downarrow$. Separating the real and imaginary parts of the eigenvalue, we obtain

$$\text{Re} \mathbf{E}(\mathbf{k}) = \gamma_e (Q^2 - K^2) + \epsilon \chi_e \gamma (Q^3 - 3QK^2) \quad \text{(A3)}$$

$$\text{Im} \mathbf{E}(\mathbf{k}) = 2 \gamma_e QK + \epsilon \chi_e \gamma (3Q^2K - K^3) \quad \text{(A4)}$$

Looking for the real-energy lines, we have the equation

$$\text{Im} \mathbf{E}(\mathbf{k}) = 0 \quad \Rightarrow \quad 2 \gamma_e Q + \epsilon \chi_e \gamma (3Q^2 - K^2) = 0 \quad \text{(A5)}$$

$$K^2 = 3Q^2 + 2 \epsilon \frac{\gamma_e}{\chi_e} Q \quad \left( = 3Q^2 + \epsilon \frac{4 \gamma_e}{\chi_e} Q \quad \text{if} \quad \mathbf{e} = e_{110} \right) \quad \text{(A6)}$$

Eq. (A6) is the relation between $Q$ and $K$ we were looking for. The energy is

$$E_e(Q) = -\epsilon 8 \chi_e \gamma Q^3 - 8 \gamma_e Q^2 - \epsilon 2 \frac{\gamma_e^2}{\chi_e} Q$$

$$= -\epsilon 4 \gamma Q^3 - 8 \gamma_e Q^2 - \epsilon 4 \frac{\gamma_e^2}{\gamma} Q \quad \text{if} \quad \mathbf{e} = e_{110} \quad \text{(A7)}$$

For a given $E(Q)$ value, we have two possible choices of $K$,

$$K = \pm \sqrt{3Q^2 + 2 \epsilon \frac{\gamma_e}{\chi_e} Q} \quad \left( = \pm \sqrt{3Q^2 + \epsilon \frac{4 \gamma_e}{\gamma} Q} \quad \text{if} \quad \mathbf{e} = e_{110} \right) \quad \text{(A8)}$$

Let us note that $|\epsilon 4 (\gamma / \gamma_e) Q| \gg 3Q^2$ so that $|Q| \ll |K|$ and

$$K \approx \pm \sqrt{(4\epsilon \gamma_c / \gamma) Q} \quad \text{(A9)}$$
The sign of $\epsilon \gamma$ determines the sign of $Q$ ($\gamma_c > 0$). As stated above $\epsilon \gamma > 0$, which corresponds to spin $\uparrow$, gives $Q > 0$ whereas $\epsilon \gamma < 0$, which corresponds to spin $\downarrow$, gives $Q < 0$.

We have the symmetry property

$$E_\pm(Q) = E_\mp(-Q)$$  \hspace{1cm}  (A10)

The study of the function $E(Q)$ is straightforward and we take $\epsilon = -1$ in the following, the other case being deduced by symmetry:

$$\frac{dE_-(Q)}{dQ} = 24X_e \gamma Q^2 - 16\gamma_c Q + 2\frac{\gamma^2_c}{\gamma X_e} \left( = 12\gamma Q^2 - 16\gamma_c Q + 4\frac{\gamma^2_c}{\gamma} \text{ if } e = e_{110} \right)$$  \hspace{1cm}  (A11)

The roots $Q_1$ and $Q_2$ of the derivative are

$$Q_1 = \frac{\gamma_c}{2\gamma X_e}, \quad Q_2 = \frac{\gamma_c}{6\gamma X_e}$$

$$Q_1 = \frac{\gamma_c}{\gamma}, \quad Q_2 = \frac{\gamma_c}{3\gamma} \text{ if } e = e_{110} \hspace{1cm}  (A12)$$

Incidentally we note that

$$E_-(Q_1) = 0 \hspace{1cm}  (A13)$$

The corresponding curve is plotted in Fig. 4. It must be realized that we are only dealing with evanescent states, which correspond to a negative energy. Thus, for a given energy $E < 0$, we have two possible $Q$-values, $\pm Q$, each associated with a given spin subband.

Finally, we find that, at a given energy, we have exactly the four possible states, the wave vectors of which are ($Q \pm iK$) with spin $\uparrow$ and ($-Q \pm iK$) with spin $\downarrow$, the latter being obtained from the former through $\hat{K}$. In short

$$E_\uparrow(k) = E_\uparrow(k^*) = E_\downarrow(-k) = E_\downarrow(-k^*) \hspace{1cm}  (A14)$$

**APPENDIX B: CONTINUITY EQUATION AND DEFINITION OF THE PROBABILITY CURRENT**

1. Definition of the probability current

Consider a Hamiltonian given by

$$\hat{H} = \sum_j a_j \hat{p}_j + \sum_{j,k} b_{jk} \hat{p}_j \hat{p}_k + \sum_{j,k,l} c_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l + V$$  \hspace{1cm}  (B1)
where $a_j$, $b_{jk}$, $c_{jkl}$ are Hermitian matrices, invariant under permutation of the indices $i$, $j$, $k$, and where $V$ is real. We define the velocity operator

$$
\hat{v}_j = \frac{\partial \hat{H}}{\partial p_j} = a_j + 2 \sum_k b_{jk}\hat{p}_k + 3 \sum_{k,l} c_{jkl}\hat{p}_k\hat{p}_l
$$

(B2)

It will be useful to take the following notations:

$$
|\psi\rangle = \psi_1(r) \uparrow + \psi_2(r) \downarrow = \begin{bmatrix} \psi_1(r) \\ \psi_2(r) \end{bmatrix},
|\phi\rangle = \phi_1(r) \uparrow + \phi_2(r) \downarrow = \begin{bmatrix} \phi_1(r) \\ \phi_2(r) \end{bmatrix}
$$

\(\psi\) = \[\psi_1^*(r) \ \psi_2^*(r)\], \(\phi\) = \[\phi_1^*(r) \ \phi_2^*(r)\], \(\phi|\psi\rangle = \phi_1^*(r)\psi_1(r) + \phi_2^*(r)\psi_2(r)

\(\langle \psi|\phi\rangle = \psi_1^*(r)\phi_1(r) + \psi_2^*(r)\phi_2(r) = |\psi|^2 = |\phi|^2

\[\hat{p}\psi\rangle = \begin{bmatrix} \hat{p}\psi_1(r) \\ \hat{p}\psi_2(r) \end{bmatrix},
\langle \hat{p}\phi|\psi\rangle = |\hat{p}\phi_1^*(r) \ \hat{p}\phi_2^*(r)| = -\hat{p}\phi_1^*(r) - \hat{p}\phi_2^*(r)

(B3)

The Schrödinger equation is

$$
i\hbar \frac{\partial |\psi\rangle}{\partial t} = \sum_j a_j\hat{p}_j |\psi\rangle + \sum_{j,k} b_{jk}\hat{p}_j\hat{p}_k |\psi\rangle + \sum_{j,k,l} c_{jkl}\hat{p}_k\hat{p}_l |\psi\rangle
$$

$$
- \frac{i\hbar}{\partial t} |\psi\rangle = \sum_j (\hat{p}_j|\psi\rangle a_j + \sum_{j,k} (\hat{p}_j\hat{p}_k|\psi\rangle b_{jk} + \sum_{j,k,l} (\hat{p}_j\hat{p}_k\hat{p}_l|\psi\rangle c_{jkl}
$$

(B4)

The continuity equation can be written

$$
i\hbar \left[ (\psi|\frac{\partial}{\partial t}|\psi\rangle + (\frac{\partial}{\partial t}|\psi|\psi\rangle \right] = i\hbar \frac{\partial |\psi\rangle^2}{\partial t}
$$

$$
= \sum_j [(\psi|a_j\hat{p}_j\psi) - (\hat{p}_j\psi|a_j\psi)]
$$

+ \sum_{j,k} [(\psi|b_{jk}\hat{p}_j\hat{p}_k\psi) - (\hat{p}_j\hat{p}_k|b_{jk}\psi)]
$$

+ \sum_{j,k,l} [(\psi|c_{jkl}\hat{p}_j\hat{p}_k\hat{p}_l\psi) - (\hat{p}_j\hat{p}_k\hat{p}_l|b_{jk}\psi)]
$$

(B5)

Note that

$$
(\psi|a_j\hat{p}_j|\psi) = (a_j\hat{p}_j|\psi)\ast = (\hat{p}_j|a_j\psi)\ast
$$

(B6)

or

$$
(\hat{p}_j|a_j\psi) = (\psi|a_j\hat{p}_j)\ast
$$

(B7)
Similarly

\[ (\hat{p}_j \hat{p}_k \psi | b_{jk} \psi) = (\psi | b_{jk} \hat{p}_j \hat{p}_k \psi)^* \quad ; \quad (\hat{p}_j \hat{p}_k \hat{p}_l \psi | b_{jk} \psi) = (\psi | c_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l \psi)^* \]  

(B8)

Therefore

\[
\frac{\partial |\psi|^2}{\partial t} = \frac{2}{h} \text{Im} \left[ \sum_j (\psi | a_j \hat{p}_j \psi) + \sum_{j,k} (\psi | b_{jk} \hat{p}_j \hat{p}_k \psi) + \sum_{j,k,l} (\psi | c_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l \psi) \right] \tag{B9}
\]

The probability current \( J \) has to satisfy

\[
\nabla \cdot J = -\frac{2}{h} \text{Im} \left[ \sum_j (\psi | a_j \hat{p}_j \psi) + \sum_{j,k} (\psi | b_{jk} \hat{p}_j \hat{p}_k \psi) + \sum_{j,k,l} (\psi | c_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l \psi) \right] = \nabla \cdot J^{(1)} + \nabla \cdot J^{(2)} + \nabla \cdot J^{(3)} \tag{B10}
\]

From the expression of the velocity operator, we tentatively define the probability current as

\[
\tilde{J}_j = \left[ \frac{1}{2} (\psi | a_j \psi) + \sum_k (\psi | b_{jk} \hat{p}_k \psi) + \frac{3}{2} \sum_{j,k,l} (\hat{p}_k \psi | c_{jkl} \hat{p}_k \psi) \right] + cc \tag{B11}
\]

where \( cc \) refers to the complex conjugate. We calculate

\[
\nabla \cdot \tilde{J} = \sum_j \nabla_j \tilde{J}_j = \frac{i}{h} \sum_j \hat{p}_j \tilde{J}_j \tag{B12}
\]

Let us consider the first term

\[
\tilde{J}^{(1)}_j = \frac{1}{2} (\psi | a_j \psi) + cc = (\psi | a_j \psi) \tag{B13}
\]

\[
\sum_j \nabla_j \tilde{J}^{(1)}_j = \frac{i}{h} \sum_j \hat{p}_j (\psi | a_j \psi) = \frac{i}{h} \sum_j (\psi | a_j \hat{p}_j \psi) - (\hat{p}_j \psi | a_j \psi) = -\frac{2}{h} \text{Im} \sum_j (\psi | a_j \hat{p}_j \psi) = \nabla \cdot J^{(1)} \tag{B14}
\]

The second term gives

\[
\tilde{J}^{(2)}_j = \sum_k (\psi | b_{jk} \hat{p}_k \psi) + cc = \sum_k [(\psi | b_{jk} \hat{p}_k \psi) + (\hat{p}_k \psi | b_{jk} \psi)] \tag{B15}
\]

\[
\sum_j \nabla_j \tilde{J}^{(2)}_j = \frac{i}{h} \sum_{j,k} [(\psi | b_{jk} \hat{p}_j \hat{p}_k \psi) - (\hat{p}_j \hat{p}_k \psi | b_{jk} \psi) + (\hat{p}_k \psi | b_{jk} \hat{p}_j \psi) - (\hat{p}_j \hat{p}_k \psi | b_{jk} \psi)]
\]

\[
= -\frac{2}{h} \text{Im} \sum_j (\psi | b_{jk} \hat{p}_j \hat{p}_k \psi) = \nabla \cdot J^{(2)} \tag{B16}
\]
Concerning to the third term
\[\tilde{J}^{(3)}_j = \frac{3}{2} \sum_{k,l} (p_k \psi|c_{jkl}\hat{p}_l \psi) + cc = 3 \sum_{k,l} (p_k \psi|c_{jkl}\hat{p}_l \psi) \tag{B17}\]
\[\sum_j \nabla_j \tilde{J}^{(3)}_j = \frac{3i}{\hbar} \sum_{k,l} [(\hat{p}_k \psi|c_{jkl}\hat{p}_j \hat{p}_l \psi) - (\hat{p}_j \hat{p}_k \psi|c_{jkl}\hat{p}_l \psi)] \neq \nabla \cdot J^{(3)} \tag{B18}\]

Let us now consider the quantity
\[\sum_{jkl} \hat{p}_j \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) = \sum_{jkl} [(\psi|c_{jkl}\hat{p}_j \hat{p}_k \hat{p}_l \psi) - (\hat{p}_j \hat{p}_k \hat{p}_l \psi|c_{jkl}\psi)]
-3 \sum_{jkl} [(\hat{p}_j \psi|c_{jkl}\hat{p}_k \hat{p}_l \psi) - (\hat{p}_j \hat{p}_k \psi|c_{jkl}\hat{p}_l \psi)]
= \sum_j \hat{p}_j \sum_{kl} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi)
= \frac{\hbar}{i} \sum_j \nabla_j \sum_{kl} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) \tag{B19}\]

We have
\[\sum_j \nabla_j \left[ \sum_{k,l} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) + \tilde{J}^{(3)}_j \right] = -\frac{2}{\hbar} \text{Im} \sum_{j,k,l} (\psi|c_{jkl}\hat{p}_j \hat{p}_k \hat{p}_l \psi) = \nabla \cdot J^{(3)} \tag{B20}\]

Thus, we can define
\[J^{(3)}_j = \tilde{J}^{(3)}_j + \sum_{k,l} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) \tag{B21}\]

Finally, the \(j\) component of the probability current can be taken as
\[J_j = \left[ \frac{1}{2} (\psi|a_j \psi) + \sum_k (\psi|b_{jk} \hat{p}_k \psi) + \frac{3}{2} \sum_{j,k,l} (\hat{p}_k \psi|c_{jkl}\hat{p}_j \hat{p}_l \psi) + \frac{1}{2} \sum_{k,l} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) \right] + cc \tag{B22}\]

or
\[J_j = J_j^f + (\psi|a_j \psi) + 3 \sum_{j,k,l} (\hat{p}_k \psi|c_{jkl}\hat{p}_j \hat{p}_l \psi) + \sum_{k,l} \hat{p}_k \hat{p}_l (\psi|c_{jkl}\psi) \tag{B23}\]

2. Quantum well grown in the [110] direction

To illustrate some simple consequences, we apply the preceding results to the practical case of quantum wells grown in the [110] direction. First, let us point out that, in this case, a direct calculation of the current of probability is straightforward
\[i\hbar \frac{\partial \psi_{\pm}}{\partial t} = -\gamma_c \frac{\partial^2 \psi_{\pm}}{\partial z^2} \pm \frac{1}{2} i\gamma \frac{\partial^3 \psi_{\pm}}{\partial z^3}\]
\[-i\hbar \frac{\partial \psi_{\mp}}{\partial t} = -\gamma_c \frac{\partial^2 \psi_{\mp}}{\partial z^2} \pm \frac{1}{2} i\gamma \frac{\partial^3 \psi_{\mp}}{\partial z^3} \tag{B24}\]
Multiplying the first equation by $\psi^*_\pm$, the second equation by $\psi_\pm$ and subtracting them, we obtain

\[ i\hbar \left( \psi^*_\pm \frac{\partial \psi_\pm}{\partial t} + \psi_\pm \frac{\partial \psi^*_\pm}{\partial t} \right) = -\gamma_c \left( \psi^*_\pm \frac{\partial^2 \psi_\pm}{\partial z^2} - \psi_\pm \frac{\partial^2 \psi^*_\pm}{\partial z^2} \right) + \frac{1}{2} i \gamma \left( \psi^*_\pm \frac{\partial^3 \psi_\pm}{\partial z^3} + \psi_\pm \frac{\partial^3 \psi^*_\pm}{\partial z^3} \right) \]

or

\[ -\nabla \cdot \mathbf{J}_\pm = \frac{\partial |\psi|^2}{\partial t} = -\gamma_c \left( \psi^*_\pm \frac{\partial^2 \psi_\pm}{\partial z^2} - \psi_\pm \frac{\partial^2 \psi^*_\pm}{\partial z^2} \right) + \frac{1}{2} \gamma \left( \psi^*_\pm \frac{\partial^3 \psi_\pm}{\partial z^3} + \psi_\pm \frac{\partial^3 \psi^*_\pm}{\partial z^3} \right) \]

\[ = -\nabla \cdot \left[ \mathbf{J}_\pm \pm \frac{\gamma}{\hbar} \left( 3 \left| \frac{\partial}{\partial z} \psi_\pm \right|^2 - \frac{\partial^2}{\partial z^2} |\psi_\pm|^2 \right) \right] \]

We consider a well made of a spin-split semiconductor (GaAs) confined between infinite walls located at $z = 0$ and $z = a$. At energy $E$, for a given spin, the wave function $\phi(z)$ consists of a combination of eigenstates associated to the wave vectors $q(E)$ and $-q'(E)$ (see Fig. 6, upper part) which satisfy

\[ \gamma_c q^2 + \frac{1}{2} \gamma q^3 = \gamma_c q'^2 - \frac{1}{2} \gamma q'^3 \]

The wave function writes

\[ \phi(z) = A e^{i qz} + B e^{-i q'z} \]

and verifies the boundary condition: $\phi(0) = \phi(a) = 0$ so that $A = -B$ and $q + q' = n \frac{2 \pi}{a}$, or

\[ \phi(z) = 2i A \sin \left( \frac{n \pi}{a} z \right) e^{-i q'z} \]

A straightforward calculation gives

\[ -\nabla \cdot \mathbf{J} = \frac{\partial |\phi|^2}{\partial t} = -\frac{2}{\hbar} |A|^2 \sin \{(q + q')z\} \left[ \gamma_c (q^2 - q'^2) + \frac{1}{2} \gamma (q^3 + q'^3) \right] = 0 \]

due to the energy expression (Eq. B27). The probability current $\mathbf{J}$ is conserved as it should. However, a calculation of $\mathbf{J}$ according to Eq. B26 yields

\[ \mathbf{J}_\pm = \pm \frac{1}{2\hbar} \gamma |A|^2 (q + q')^2 \]

Obviously, we should have $\mathbf{J}_\pm = 0$. This inconsistency arises due to a lack in the modelization relative to the singular case of infinite wall. Note that, if dealing with a finite barrier, $(\gamma/2\hbar) |A|^2 (q + q')^2 = (2\gamma_c/\hbar) |A|^2 Q (q + q')^2 /K^2$, where $q$ and $Q$ are small. In the case of an infinite well, we are in a situation where $K$ tends to infinity. Because of this
inconsistency (the infinite well cannot meet the criteria used in our approximations), this term should certainly be discarded. The problem can also be circumvented when building the function

$$\Phi = \phi \uparrow + \tilde{K} (\phi \uparrow) = \phi \uparrow + \phi^* \downarrow = 2 \sin \left(\frac{n\pi}{a} z\right)[iAe^{-i\delta qz} \uparrow + (iA)^* e^{i\delta qz} \downarrow]$$

(B32)

which properly describes a solution with a spin lying in the plane perpendicular to the DP field and for which J = 0.

**APPENDIX C: [100]-Oriented Barrier, Zeroth-Order Wave-Function Coefficients**

The continuity of the wave function defined by Eqs. 4.12 and of its derivative at z = 0 and z = a for the two spin channels provides the following linear system:

$$\begin{align*}
-B_1 + A_2 + B_2 - \frac{i\xi}{2K'} \tilde{A}_2 + \frac{i\xi}{2K} \tilde{B}_2 &= A_1 \\
\frac{i}{K} B_1 - A_2 + B_2 + \frac{i\xi}{2K} \tilde{A}_2 + \frac{i\xi}{2K} \tilde{B}_2 &= i\frac{q}{K} \tilde{A}_1 \\
A_2 e^{-K_a} + B_2 e^{K_a} - \frac{i\xi}{2K'} \tilde{A}_2 e^{-K'_{a}} + \frac{i\xi}{2K} \tilde{B}_2 e^{K'_{a}} - A_3 e^{iqa} &= 0 \\
-A_2 e^{-K_a} + B_2 e^{K_a} - \frac{i\xi}{2K} \tilde{A}_2 e^{-K'_{a}} + \frac{i\xi}{2K} \tilde{B}_2 e^{K'_{a}} - i\frac{q}{K} A_3 e^{iqa} &= 0 \\
-B_{1} + \frac{i}{K} \tilde{B}_1 - A_2 + B_2 + \tilde{A}_2 + \tilde{B}_2 &= \tilde{A}_1 \\
\frac{i}{K} \tilde{B}_1 - \frac{i\xi}{2K'} \tilde{A}_2 - \frac{i\xi}{2K'} \tilde{B}_2 - \tilde{A}_2 + \tilde{B}_2 &= i\frac{q}{K} \tilde{A}_1 \\
\frac{i\xi}{2K} A_2 e^{-K_a} - \frac{i\xi}{2K} B_2 e^{K_a} + \tilde{A}_2 e^{-K'_{a}} + \tilde{B}_2 e^{K'_{a}} - \tilde{A}_3 e^{iqa} &= 0 \\
-\frac{i\xi}{2K'} A_2 e^{-K_a} - \frac{i\xi}{2K'} B_2 e^{K_a} - \tilde{A}_2 e^{-K'_{a}} + \tilde{B}_2 e^{K'_{a}} - i\frac{q}{K} \tilde{A}_3 e^{iqa} &= 0
\end{align*}$$

(C1a)-(C1h)

The coefficients A1 and $\tilde{A}_1$ which define the intensity of the two spin components of the incident wave are known (initial conditions). It could be verified that the determinant of this system is non zero. We can calculate the eight coefficients $B_1$, $\tilde{B}_1$, $A_2$, $B_2$, $\tilde{A}_2$, $\tilde{B}_2$, $A_3$, and $\tilde{A}_3$ from the eight relations, Eqs. C1. We begin to solve these eight equations to the zeroth order in $\xi/K_0$ or, in other words, by writing $\xi/K_0 = 0$. We note the eight equations are then divided into two sets: The first four equations are uncoupled to the last four ones.

The first four equations are related to the spin $[11]^t$ and write as:
\[ A_1 = -B_1 + A_2 + B_2 \] \hspace{1cm} (C2a)

\[ iqA_1 = iqB_1 - KA_2 + KB_2 \] \hspace{1cm} (C2b)

\[ A_3 e^{iqa} = A_2 e^{-Ka} + B_2 e^{Ka} \] \hspace{1cm} (C2c)

\[ iqA_3 e^{iqa} = -KA_2 e^{-Ka} + KB_2 e^{Ka} \] \hspace{1cm} (C2d)

and the last four ones are related to the spin \([1 - 1]^t\). The equations are the same by altering \((A_1, B_1, A_2, B_2, K)\) into \((\tilde{A}_1, \tilde{B}_1, \tilde{A}_2, \tilde{B}_2, K')\).

This is the usual formulation of the tunnel effect. Because Eqs. \(\text{C1}\) are written to the first order in \(\xi/K_0\), we are looking for a solution to the same order.

To give an example, we look for the results when the incident wave has a spin \([1 1]^t\) \((A_1 \neq 0, \tilde{A}_1 = 0)\). Considering Eqs. 2.25, we note that the approximation given by the last term of each equation is almost valid as soon as \(Ka > 2\). In Ref. 13, \(K\) is of the order of 0.1 Å\(^{-1}\) which gives \(a\) of the order of 20 Å in order that the inequality holds, a value which is quite reasonable.

As \(\tilde{A}_1 = 0\), this shows that to the zeroth order in \(\xi/K_0\), the results may be summarized by

\[ A_2/A_1 = f_2^{(0)} \quad \tilde{A}_2 = 0 \]
\[ A_3/A_1 = f_3^{(0)} \quad \tilde{A}_3 = 0 \]
\[ B_1/A_1 = g_1^{(0)} \quad \tilde{B}_1 = 0 \]
\[ B_2/A_1 = g_2^{(0)} \quad \tilde{B}_2 = 0 \] \hspace{1cm} (C3)

where \(f_j^{(0)} = f_j^{(0)}(q, K)\) and \(g_j^{(0)} = g_j^{(0)}(q, K)\) correspond to the standard case (Subsec. 11D) and can be deduced from Eqs. 2.25. This means that, up to the first order in \(\xi/K_0\), the results are of the shape:

\[ A_2/A_1 = f_2^{(0)} + (\xi/K) f_2^{(1)} \quad \tilde{A}_2/A_1 = (\xi/K) \tilde{f}_2^{(1)} \]
\[ A_3/A_1 = f_3^{(0)} + (\xi/K) f_3^{(1)} \quad \tilde{A}_3/A_1 = (\xi/K) \tilde{f}_3^{(1)} \]
\[ B_1/A_1 = g_1^{(0)} + (\xi/K) g_1^{(1)} \quad \tilde{B}_1/A_1 = (\xi/K) \tilde{g}_1^{(1)} \]
\[ B_2/A_1 = g_2^{(0)} + (\xi/K) g_2^{(1)} \quad \tilde{B}_2/A_1 = (\xi/K) \tilde{g}_2^{(1)} \] \hspace{1cm} (C4)

where the factors of \(f_j^{(1)} = f_j^{(1)}(q, K, K')\), \(g_j^{(1)} = g_j^{(1)}(q, K, K')\), \(\tilde{f}_j^{(1)} = \tilde{f}_j^{(1)}(q, K, K')\), and \(\tilde{g}_j^{(1)} = \tilde{g}_j^{(1)}(q, K, K')\) may be equal to zero. In fact, a calculation up to the first order in \(\xi/K_0\)
via Eqs. (C1) involves terms of \((\xi/K)\bar{A}_2\) type, which are of second-order in \(\xi/K_0\). Therefore \(f_j^{(1)} = g_j^{(1)} = 0\) and Eqs. (C4) write as

\[
\begin{align*}
A_2/A_1 &= f_2^{(0)} + (\xi/K)^2 f_2^{(2)} & \bar{A}_2/A_1 &= (\xi/K) \bar{f}_2^{(1)} \\
A_3/A_1 &= f_3^{(0)} + (\xi/K)^2 f_3^{(2)} & \bar{A}_3/A_1 &= (\xi/K) \bar{f}_3^{(1)} \\
B_1/A_1 &= g_1^{(0)} + (\xi/K)^2 g_1^{(2)} & \bar{B}_1/A_1 &= (\xi/K) \bar{g}_1^{(1)} \\
B_2/A_1 &= g_2^{(0)} + (\xi/K)^2 g_2^{(2)} & \bar{B}_2/A_1 &= (\xi/K) \bar{g}_2^{(1)} \\
\end{align*}
\]  

(C5)

where \(f_j^{(2)} = f_j^{(2)}(q, K, K')\) and \(g_j^{(2)} = g_j^{(2)}(q, K, K')\).

Of course if \(A_1 = 0\) and \(\bar{A}_1 \neq 0\), the results are to be inverted. \(f_j^{(2)}\) (resp. \(g_j^{(2)}\)) is comparable to, or smaller than, \(f_j^{(0)}\) (resp. \(g_j^{(0)}\)). In Sec. (C) it is shown that \(\bar{f}_j^{(1)} A_1\) is of the order of \(A_j\) and \(\bar{g}_j^{(1)} A_1\) is of the order of \(B_j\).
FIG. 1. Sketch of the tunnel geometry with definition of notations. The spin-orbit-split barrier material of thickness $a$ (medium II) is located between two free-electron like materials (media I and III). The tunnel axis, normal to the barrier, is the $z$ axis. In the free-electron-like materials, the real electron wave vector in the $z$ direction is referred to as $q$. In the barrier material, the evanescent wave vector along the $z$ axis is referred to as $Q + iK$, where $Q$ and $K$ are real quantities. The transverse wave vector component, in the barrier plane, $\xi$ is conserved in the tunnel process. Then, the overall wave vectors in the three media are respectively $k_I = k_{III} = \xi + q$ and $k_{II} = \xi + Q + iK$.

FIG. 2. This figure illustrates transformations which, starting from a state of wave vector $k$ and with a mean value of the Pauli operator $\langle \hat{\sigma} \rangle$, construct degenerate states. $\hat{K}_0$ is the complex conjugation and $\hat{K} = -i\sigma_y \hat{K}_0$ is the Kramers time-reversal operator. $\hat{K}$ yields a state with the wave vector $-k^*$ and with the mean spin $-\langle \hat{\sigma} \rangle$. The state of wave vector $k^*$ may be associated to another spin state, corresponding to the mean value $\langle \hat{\sigma} \rangle'$. Applying $\hat{K}$ to this state, we form a degenerate state with the wave vector $-k$ and associated to the mean spin $-\langle \hat{\sigma} \rangle'$. Four states are finally obtained.

FIG. 3. Plot of the real-energy lines inside the gap for $k = [\xi, 0, iK]$, where $K$ and $\xi$ are real and positive and $\tan \theta = \xi/K$. The calculation is performed using a $14 \times 14$ $k \cdot p$ Hamiltonian. The loops are drawn versus $||k||$ in $2\pi/a_0$ units, where $a_0$ is the cubic lattice parameter. In all these directions, the spin degeneracy is lifted. Their shape and extension sharply depend on $\theta$. For $\theta = 43.2^\circ$, the two branches are too close to be resolved at this scale. The parameters used in the calculation are: $P = 9.88$ eVÅ, $P' = 0.41$ eVÅ, $E_G = 1.519$ eV, $\Delta_c = E_{\Gamma}\Sigma_c - E_{\Gamma}\Sigma_c = 0.171$ eV, $P_X = 8.68$ eVÅ, $\Delta = 0.341$ eV, $E_\Delta = E_{\Gamma7c} - E_{\Gamma6c} = 2.969$ eV, $\Delta' = -0.17$ eV (see Ref. 30 for a complete discussion). Inset: Real-band structure (left, dashed line). For clarity, only a valence band which is connected to the evanescent branch is drawn) and evanescent band across the band gap (right, full line) along the [001] direction ($\theta = 0$) where the DP “exchange” field is zero (no spin splitting).

FIG. 4. Mathematical plot of the real-energy lines for $k$ along [110] as a function of the real part of the wave vector $Q$ in the barrier. The calculation is performed for a ratio $\gamma/\gamma_c = 0.438$ Å. We are only concerned with negative energies, which refer to evanescent states. More precisely, the physical states are located within a very small energy domain.
below the origin. The domain $Q > 0$ refers to up-spin states, whereas the domain $Q < 0$
refers to down-spin states. In each case, the imaginary component of the wave vector can
take the values $\pm K$. Thus, at a given energy, we have exactly the four possible states
$(Q \pm iK) \uparrow$ and $(-Q \pm iK) \downarrow$. The down-spin states are Kramers conjugates of the up-spin
states.

FIG. 5. This figure is a special case of Fig. 2, when the DP field $\chi$ lies along a real
direction $\mathbf{n}$. Following the same procedure, four degenerate states are constructed, which
now have their spins quantized along the same direction $\mathbf{n}$ (i.e. $\langle \hat{\sigma} \rangle = \langle \hat{\sigma}' \rangle$).

FIG. 6. (Color online). The lower part of this figure illustrates the spin-dependent tun-
neling scheme in the case of a [001] oriented barrier (Perel's case). The horizontal plane
describes the electron wave vector in the barrier; $\mathbf{K}$ is taken along the [001] axis and $\xi$ lies
in the barrier plane, along [100]. The upper part of the figure ($E > 0$) corresponds to the
real conduction band - the wave vectors are real quantities - and the parabola-like curves
describing spin-split states along the [101]-direction are drawn. An up-spin state (full line,
open circle) with the wave vector $\mathbf{q}'$ is degenerate with a down-spin state at the wave vector
$\mathbf{q}$ (dotted line, dark circle) and also with up- and down-spin states at the wave vectors $-\mathbf{q}$
and $-\mathbf{q}'$ respectively. This is useful for the calculation of a quantum well, given in Appendix
B2. Concerning the evanescent states, in a naive effective-mass picture, one may think of
evanescent states being mirrors of these real states (in the $E < 0$ domain) with imaginary
wave vectors. Then up- and down-spin electrons at the energy $E$, would tunnel with the
two different wave vectors $i\mathbf{q}'$ and $i\mathbf{q}$, thus resulting in a spin-filter effect. However, our
calculation shows that, concerning evanescent states (lower part of the figure, $E < 0$), the
situation is not so simple. In the negative-energy region, the $\mathbf{K}$ axis refers to the imaginary
wave-vector component and $\xi$ refers to the real wave-vector component. Real-energy lines
are found only when $\tan \theta = \xi/K < 1$. These real-energy lines, when drawn for a given $\theta$,
consist of loops connecting opposite spin states at the zone center ("up" spin: Full curve;
"down" spin: Dotted curve. Obviously, when going off the zone center, the spin no longer
remains a good quantum number - in fact, it can be calculated that its average value rotates
along the loop - but it has to be pointed out that, in the D'yakonov and Perel’ description,
the energy eigenvectors are also pure spin states which depend on the $\theta$ ratio). Two of these
loops are drawn here. Let us consider a tunneling process at the energy $E$ (horizontal grey
plane or yellow plane in the online edition) of an electron with the wave vector component
\( \xi \) in the barrier plane, which has to be conserved in the tunneling process. It can be observed here that the two states marked on the loops by a dark circle \((K')\) and an open circle \((K)\) - which are energy degenerate - are associated to the same real wave-vector component \( \xi \). However, they correspond to two different \( \theta \) as they are respectively associated to the imaginary components \( iK \) and \( iK' \), along the tunneling direction. The difference between \( K \) and \( K' \) results in a spin-filter effect. Inset (upper left): Top view of the plane at energy \( E \) showing the intercepts with the loops which determine the relevant wave vectors \( K \) and \( K' \).
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