

CONTROL OF TWO-DIMENSIONAL ELECTRON SPIN BY AN ABRUPT CHANGE OF PHYSICAL PARAMETERS OF A QUANTUM WELL

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We apply Clifford algebra to investigate 2D electron spin reflection off and transmission through a stepped discontinuity of physical parameters in semiconducting quantum well. The discontinuity may be due to change of spin-orbit interaction constants, effective masses, or electrostatic potential. In the paper the posed problem has been solved exactly. It is shown that the reflected electronic beam has identical spin polarization as the incident one. However, the transmitted beam suffers spin flipping and in general case consists of a mixture of up and down spin states. Optimal conditions for total reversion of 2D electron spin polarization are found. Special attention is paid to correct boundary conditions in the presence of spin-orbit interaction. A simple formula that connects spin polarization of the transmitted beam and SO interaction constants is presented.

Keywords: Clifford algebra, geometric algebra, semiconductors, spintronics, spin polarization, spin flipping, quantum well

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1. Introduction

The Clifford (geometric) algebra is a noncommutative algebra which is especially suitable for description of rotations in multidimensional spaces having positive, negative, or mixed signatures. Two of them, $Cl_{3,0}$ and $Cl_{1,3}$, are used to describe classical and relativistic physics. At present there has appeared a number of introductory books on Clifford algebra [1–3] as well as specialized books on classical mechanics [4], electrodynamics [5, 6], relativity theory [7], cosmology [8], computer vision and robotics [9] to mention a few only. Also a number of books on Clifford calculus have been published [10, 11].

Recently the first attempt to adapt the Clifford algebra to semiconductor physics was made [12–18]. In the papers [12–16], electron and hole spin precession in bulk cubic semiconductors A_3B_5 and A_2B_6 was considered in terms of multivectors. It was shown that for the description of spin-split conduction band and electron spin precession the most suitable is $Cl_{3,0}$ Clifford algebra. For more complicated valence bands, two algebras – $Cl_{4,0}$ and mixed signature $Cl_{4,1}$ – were addressed. The equivalence rules between the Hilbert space and Clifford algebra formulations of quantum mechanics were obtained. In papers [17, 18], spin reflection in 2D

and 3D semiconductors for electrons obliquely incident onto an infinite potential barrier was analysed. It has been shown that apart from ordinary electronic wave an extraordinary one appears if electron is incident at an angle to a flat potential barrier. The interference of the incident beam with the reflected ordinary and extraordinary beams that propagate at different angles to barrier normal results in a spatial interference pattern having two characteristic spatial beating periods.

Till now, spin flipping in semiconductors was considered under simplified boundary conditions. The incident electron was assumed to be in spin-degenerate bands while the spin-orbit (SO) interaction was included in the barrier region only [19–21], or infinite boundary conditions were used [16, 18]. In all cases the spin-flipping occurs only for electrons obliquely incident onto the barrier. This is difficult to control experimentally, or a special sample configuration is needed [22]. In this paper we shall show that one can achieve spin flipping in a quantum well (QW) at vertical incidence of beam onto barrier as well, if SO interaction is included on both sides of the discontinuity and correct boundary condition are taken into account.

Recently an attempt to solve a nonrelativistic Schrödinger equation in the presence of square quaternionic potentials was undertaken by De Leo et al. [23–26].

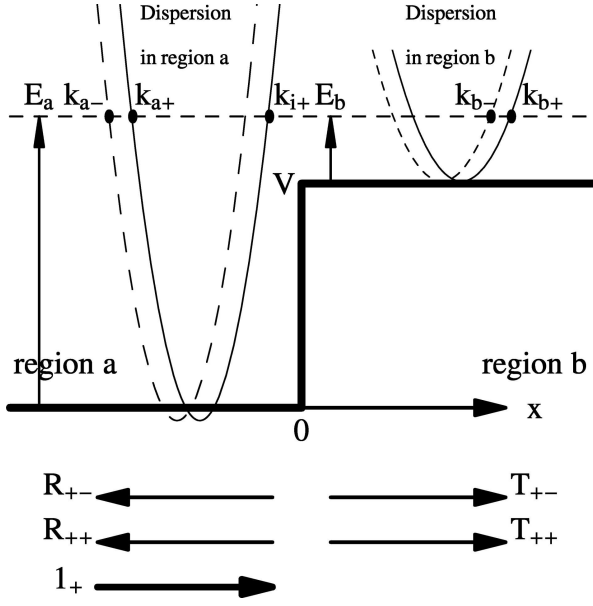


Fig. 1. Thick line shows the potential step of height V . In the lower part of the figure, the horizontal lines show the incident wave of unit amplitude $1_+ = \psi_+$, reflected, and transmitted ordinary ($++$) and extraordinary ($+ -$) waves. In the upper part, thin solid and dashed lines show electron dispersions for up and down spin states described by Eq. (9), where characteristic wave vectors (incident wave vector k_{i+} , reflected k_{a+} , k_{a-} , and transmitted k_{b+} , k_{b-}) are shown by dots. The kinetic energies E_a and E_b in the conduction bands in regions a and b are indicated by vertical arrows.

These interesting papers demonstrate a different analytical approach to application of noncommutative quaternionic algebra to electron diffusion problem. The quaternions, as known, constitute an even subalgebra of $Cl_{3,0}$. The present work shows that it is more convenient to address to full $Cl_{3,0}$ algebra and to formulate the problems in terms of scalars, vectors, bivectors, and pseudoscalars [3] rather than to adjust the problem to a Procrustes bed of quaternions. The quaternionic Hamiltonian used in papers [23–26] here, as it is accepted in semiconductor physics, will be called spin-orbit Hamiltonian, or Rashba and Dresselhaus Hamiltonian if it is necessary to indicate a specific SO interaction mechanism.

2. $Cl_{3,0}$ Hamiltonian and spin

We shall consider the QW that is grown on (100) plane of a cubic semiconductor. The QW consists of two regions a and b where physical parameters may be different, Fig. 1. As shown by the dashed and solid parabolic-like lines in the figure, the degenerate conduction band is assumed to be spin-split by either Rashba or Dresselhaus SO interactions, or both SO mechanisms acting simultaneously, the strength of

which is characterized by constants $\alpha_{\mathbf{R}}$ and $\alpha_{\mathbf{D}}$. If the QW is fabricated from the same material (homobarrier) the SO interaction constants may be controlled by external voltage applied to a split-electrode deposited on QW plane. If constituting materials of regions a and b are different, we have the heterobarrier. In the latter case the potential step V may appear between regions a and b . Also, the SO interaction can be controlled by interface charge trapped in walls of the QW.

In the Clifford algebra the time-dependent Schrödinger equation for a spinor Ψ in the conduction band of semiconductor has the following form:

$$\hbar \frac{\partial \Psi}{\partial t} I \sigma_3 = H(\Psi). \quad (1)$$

The appearance of bivector $I \sigma_3 = \sigma_1 \sigma_2 = -\sigma_2 \sigma_1$ indicates that the quantization axis is parallel to vector σ_3 . In a cubic crystal the bivector $I \sigma_3$ represents (001) orientated crystal plane. The vector σ_3 is perpendicular to this plane. The remaining equivalent crystal planes are represented by bivectors $I \sigma_1$ and $I \sigma_2$. The presence of pseudoscalar $I = \sigma_1 \sigma_2 \sigma_3$ indicates the duality of the elements. For example, σ_3 and $I \sigma_3$ are mutually dual elements which respectively represent unit vector and oriented unit plane that is perpendicular to σ_3 . In Eq. (1) the Hamiltonian function consists of kinetic, potential barrier, and SO interaction energies,

$$H(\Psi) = -\frac{\hbar^2}{2m^*} \nabla^2 \Psi + V(\mathbf{x}) \Psi + H_{\text{SO}}(\Psi). \quad (2)$$

In this paper the potential $V(\mathbf{x})$ is considered to be a scalar rather than a quaternion. In $Cl_{3,0}$ the nabla operator has the form $\nabla = \sigma_1 \frac{\partial}{\partial x} + \sigma_2 \frac{\partial}{\partial y} + \sigma_3 \frac{\partial}{\partial z}$. The SO interaction function is

$$H_{\text{SO}}(\Psi) = (\varepsilon_1 \sigma_1 + \varepsilon_2 \sigma_2 + \varepsilon_3 \sigma_3) \Psi \sigma_3, \quad (3)$$

where the scalar coefficients ε_i depend on a particular SO interaction mechanism. Since the Clifford algebra is noncommutative, the order of different multipliers in the multivector is important.

For stationary states characterized by energy E the spinor solution can be separated into coordinate and time-dependent parts:

$$\Psi = \psi(\mathbf{x}) e^{-I \sigma_3 E t / \hbar}. \quad (4)$$

Insertion of Ψ into the Schrödinger equation (1) gives stationary equation for spinor $\psi(\mathbf{x})$,

$$-\frac{\hbar^2}{2m^*} \nabla^2 \psi + V \psi + \varepsilon \psi \sigma_3 = E \psi, \quad (5)$$

where we have introduced the vector with projections ε_i ,

$$\varepsilon = \varepsilon_1 \sigma_1 + \varepsilon_2 \sigma_2 + \varepsilon_3 \sigma_3. \quad (6)$$

In the Clifford algebra formulation, similarly as in the standard quantum mechanics formulation, the spectrum of a quantum system is found from the eigenvalue equation. In the Clifford algebra the corresponding equation reads:

$$H(\psi_{\pm}) = E_{\pm} \psi_{\pm}, \quad (7)$$

where E_{\pm} and ψ_{\pm} are the eigenenergies and eigenspinors, respectively, for up (+) and down (–) spin states. Since the multipliers in the Clifford algebra do not commute and the eigenspinor may appear to be squeezed between elementary vectors, bivectors, etc. (compare Eq. (3)), the Hamiltonian in (7) is written as a function of the eigenspinor rather than a product of operator and spinor as it is in the standard quantum mechanics. For (001) quantum well the coefficients in (6) are

$$\begin{aligned} \varepsilon_1 &= k_x \alpha_D + k_y \alpha_R, \\ \varepsilon_2 &= -k_x \alpha_R - k_y \alpha_D, \\ \varepsilon_3 &= 0. \end{aligned} \quad (8)$$

In the following we shall limit ourselves to a normal electron incidence onto a stepped discontinuity. Then the components of electron wave vector are $k_x \equiv k$ and $k_y = 0$. In experiment this condition can be satisfied if the QW in y direction is narrow enough. In the following it is also assumed that $V = 0$ in the region a while V is constant in the region b . The eigenenergies in regions a and b that follow from the eigenvalue equation and Hamiltonian then are

$$\begin{aligned} E_{a\pm} &= \frac{\hbar^2 k^2}{2m_a^*} \mp \alpha_a k, \\ E_{b\pm} &= \frac{\hbar^2 k^2}{2m_b^*} + V \mp \alpha_b k, \end{aligned} \quad (9)$$

where effective SO interaction constants were introduced, $\alpha_a = \sqrt{\alpha_{D_a}^2 + \alpha_{R_a}^2}$ and $\alpha_b = \sqrt{\alpha_{D_b}^2 + \alpha_{R_b}^2}$. The plus and minus signs correspond to spin-split energy subbands as shown in Fig. 1. The respective eigenspinors that correspond to these eigenenergies are

$$\psi_{a\pm} = \frac{\mp 1}{\sqrt{2} \alpha_a} (\alpha_{D_a} \pm \alpha_a I \sigma_2 + \alpha_{R_a} I \sigma_3),$$

$$\psi_{b\pm} = \frac{\mp 1}{\sqrt{2} \alpha_b} (\alpha_{D_b} \pm \alpha_b I \sigma_2 + \alpha_{R_b} I \sigma_3). \quad (10)$$

They are normalized, $\tilde{\psi}_{a+} \psi_{a+} = \tilde{\psi}_{a-} \psi_{a-} = 1$ and $\tilde{\psi}_{b+} \psi_{b+} = \tilde{\psi}_{b-} \psi_{b-} = 1$, where the tilde indicates the reversion operation. The orthogonality is satisfied if only the scalar part of the product is understood, $\langle \tilde{\psi}_{a+} \psi_{a-} \rangle = \langle \tilde{\psi}_{b+} \psi_{b-} \rangle = 0$. However, in general the product of different eigenspinors gives the bivector, for example, $\tilde{\psi}_{a+} \psi_{a-} = \alpha_a^{-1} (\alpha_{D_a} I \sigma_2 - \alpha_{R_a} I \sigma_1)$.

There exists the following replacement rule between a spinor defined in the Hilbert space and spinor in a vector space of $Cl_{3,0}$, i.e. the Pauli column spinor $|\psi\rangle$ is placed in one-to-one correspondence with a 4-component quaternion of the Clifford algebra via relation [3, 15]

$$\begin{aligned} |\psi\rangle &= \begin{bmatrix} a_0 + i a_3 \\ -a_2 + i a_1 \end{bmatrix} \longleftrightarrow \psi = \\ &a_0 + a_1 I \sigma_1 + a_2 I \sigma_2 + a_3 I \sigma_3, \end{aligned} \quad (11)$$

where $i = \sqrt{-1}$, and all a_i s are real numbers. The spinor ψ is isomorphic to quaternion. If the rule (11) is applied to the eigenspinor (10) in the region a , one finds the following Hilbert space ket-vector:

$$|\psi_{a\pm}\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} \pm e^{i \arctan(\alpha_{R_a}/\alpha_{D_a})} \\ 1 \end{bmatrix}. \quad (12)$$

In general there are many eigenspinors in the Hilbert space that satisfy a given eigenvalue equation. This is also true for Clifford algebra and Eq. (7). One can construct a more general eigenspinor of the Hamiltonian (5) in a form of pure bivector, namely,

$$\psi'_{\pm} = -\frac{I(\varepsilon \pm \varepsilon \sigma_3)}{\sqrt{2\varepsilon(\varepsilon \pm \varepsilon_3)}}, \quad \tilde{\psi}'_{\pm} \psi'_{\pm} = 1, \quad (13)$$

which is defined in coordinate independent way and which also satisfies the eigenvalue equation (7) with eigenenergies (9). Here $\varepsilon = |\varepsilon| = \sqrt{\varepsilon \varepsilon} = \sqrt{\varepsilon \tilde{\varepsilon}}$ is the magnitude of the vector ε . The unit vector σ_3 indicates the direction of the quantization axis which, in general, may be pointing in any arbitrary direction. As mentioned earlier, the vector σ_3 in a cubic semiconductor is along [001] axis. As we shall see, selection of a concrete vector ε fixes the direction of the average electron spin in space with respect to crystallographic axes. If coordinates from Eq. (8) are inserted into spinor (13)

and effective SO constant $\alpha = \sqrt{\alpha_R^2 + \alpha_D^2}$ is introduced, the equation (13) becomes

$$\psi'_{\pm} = \frac{1}{\sqrt{2}\alpha}(-\alpha_D I\sigma_1 + \alpha_R I\sigma_2 \mp \alpha I\sigma_3), \quad (14)$$

which differs from the eigenspinors (10). Nonetheless the eigenspinors (10) and ψ'_{\pm} give the same physically measurable quantities. In particular, they yield the same dispersion relations and average electron spin (17), albeit with opposite spin direction and interchanged spectrum branches. In $Cl_{3,0}$ algebra the measured average spin vector is calculated in the following way [3, 15]:

$$\mathbf{s} = \psi \sigma_3 \tilde{\psi}. \quad (15)$$

Since in the Clifford algebra the spinor ψ at the same time represents a rotor, the physical interpretation of Eq. (15) is very lucid: at first one aligns the spin along the quantization axis, which is parallel to σ_3 , and then with the help of spinor ψ rotates it to the true direction. The concrete expression for rotor ψ follows from the Schrödinger equation (5). If one inserts the coordinate independent spinor (13) into expression (15), one gets the following average spin:

$$\mathbf{s}_{\pm} = \psi'_{\pm} \sigma_3 \tilde{\psi}'_{\pm} = \pm \frac{\boldsymbol{\varepsilon}}{\sqrt{\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}}} = \pm \frac{\boldsymbol{\varepsilon}}{\varepsilon}. \quad (16)$$

Here the dot indicates the scalar product of vectors \mathbf{a} and \mathbf{b} defined via geometric product as $\mathbf{a} \cdot \mathbf{b} = (\mathbf{ab} + \mathbf{ba})/2$. When $\mathbf{a} = \mathbf{b}$ then $\mathbf{a} \cdot \mathbf{b} = \mathbf{ab} = \tilde{\mathbf{a}}\mathbf{b} = \mathbf{a}\tilde{\mathbf{b}}$. The expression (16) shows that the vector $\boldsymbol{\varepsilon}$ in the Hamiltonian (5) defines an average and experimentally measurable electron spin¹. In the considered case of normal incidence we have $\varepsilon_1 = k_x \alpha_D$, $\varepsilon_2 = -k_x \alpha_R$, $\varepsilon_3 = 0$. Then Eq. (16) reduces to

$$\mathbf{s}_{\pm} = \pm \frac{\alpha_D \sigma_1 - \alpha_R \sigma_2}{\sqrt{\alpha_R^2 + \alpha_D^2}}, \quad (17)$$

which shows that in the presence of Rashba and Dresselhaus interactions the spin vector lies in the quantum well plane. The spin direction is determined by relative strength of SO interaction constants. The same expression is found if instead of (14), which is a pure bivector, one inserts one of the spinors (10). Only the signs before the spin vector will be different in the final result. One also can verify that the spin-split energy branches are mutually interchanged in the states (10) and (14). Physically this has no consequences, since

¹ To have dimensional quantities the spin should be multiplied by $\hbar/2$.

which of the energy branches will represent spin-up direction (equivalently plus sign) is a matter of convention. In the following we shall use eigenspinors given by expression (10).

3. Kramers (time reversal) operator and unitarity in $Cl_{3,0}$

The Kramers operator frequently appears when one is dealing with degenerate energy bands and SO interaction. In Hilbert space formulation of quantum mechanics the Kramers operator for 1/2 spin is defined as [27]

$$\hat{K} = -i\hat{\sigma}_y K_0, \quad (18)$$

where K_0 is the complex conjugation operation. The Kramers operator \hat{K} commutes with the degenerate part of the Hamiltonian. Under action of \hat{K} the energies remain doubly degenerate (invariant of the system). In the Clifford algebra the Kramers operator goes to Kramers function

$$\hat{K}|\psi\rangle \longleftrightarrow K(\psi) = -\psi I\sigma_2. \quad (19)$$

The appearance of vector σ_2 here indicates the gauge invariance, i. e. the requirement that the physics is unaffected by alignment of σ_1 and σ_2 vectors in $I\sigma_3$ plane. As follows from the rule (11), the spin up and down states referenced with respect to quantization axis correspond to elementary scalar and bivector,

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \longleftrightarrow 1, \quad \begin{bmatrix} 0 \\ 1 \end{bmatrix} \longleftrightarrow -I\sigma_2. \quad (20)$$

Application of the Kramers function to these states yields

$$K(1) = -I\sigma_2, \quad K(-I\sigma_2) = -1, \quad (21)$$

i. e. up to the sign the Kramers operator interchanges up and down spin states. Thus, the application of the Kramers operator to one of the eigenstates allows one to construct the second linearly independent state, which customarily is called the Kramers state. For example, one finds that

$$K(\psi_{a+}) = \frac{1}{\sqrt{2}\alpha_a}(-\alpha_a + \alpha_{R_a} I\sigma_1 + \alpha_{D_a} I\sigma_2), \quad (22)$$

which is orthogonal to the initial state

$$\tilde{\psi}_{a+} K(\psi_{a+}) = 0. \quad (23)$$

The spinor (22) is different from the partner spinor defined by (10) and used in the present paper. It should be also noted that now the orthogonality condition (23)

is exact, i. e. the bivector part does not appear in the product of the eigenspinors.

A few words about unitary transformation in $Cl_{3,0}$. In the Hilbert space the unitary operator transforms spinor to another spinor. So, it can be employed to describe the evolution of the quantum system in time. Similar operator can be defined in the Clifford algebra [3], although its role here is less important since ψ , being a rotor and spinor simultaneously, controls the evolution of the spin vector. The multivector M is said to be unitary if it satisfies $|M| = \sqrt{M\tilde{M}} = \sqrt{\tilde{M}M} = 1$. Thus, in the Clifford algebra all normalized spinors are unitary, $\psi\tilde{\psi} = 1$. In $Cl_{3,0}$ they form $SU(2)$ rotation group under multiplication. In particular, multiplication of the spinor by phase factor is also the unitary transformation,

$$\psi \rightarrow \psi e^{\phi I\sigma_3} = \psi(\cos \phi + I\sigma_3 \sin \phi). \quad (24)$$

When $\phi = \pi/2$ the phase transformation is equivalent to multiplication by $I\sigma_3$. For example, if ψ'_\pm is right multiplied by phase factor $\pm I\sigma_3$ and then the Kramers' conjugation is applied, one returns to initial ψ_\pm given by Eq. (10).

The unitary transformation can be employed to bring Rashba Hamiltonian to Dresselhaus Hamiltonian and vice versa. Two-dimensional Rashba and Dresselhaus Hamiltonian functions can be obtained from Eqs. (3) and (8). They are

$$H_R(\psi) = (k_y\alpha_R\sigma_1 - k_x\alpha_R\sigma_2)\psi\sigma_3, \quad (25)$$

$$H_D(\psi) = (k_x\alpha_D\sigma_1 - k_y\alpha_D\sigma_2)\psi\sigma_3. \quad (26)$$

The unitary transformation that connects them has the following form:

$$U(\psi) = \frac{1}{\sqrt{2}}(\sigma_1 + \sigma_2)\psi\sigma_3. \quad (27)$$

The mutual transformation between Rashba and Dresselhaus Hamiltonians can be checked by calculating the identity

$$H_D(U(\psi)) = U(H_R(\psi))\Big|_{\alpha_R \rightarrow -\alpha_D} \quad (28)$$

for an arbitrary spinor in $Cl_{3,0}$. The identity (28) is equivalent to the Hilbert space transformation $\hat{H}_D\hat{U}|\psi\rangle = \hat{U}\hat{H}_R|\psi\rangle$. Also, with the help of (27) and (28) it can be demonstrated that the transformation (27) is no more than coordinate transformation: $\sigma_1 \rightarrow \sigma_2$, $\sigma_2 \rightarrow \sigma_1$, $\sigma_3 \rightarrow -\sigma_3$. However, when both the Rashba and Dresselhaus SO mechanisms are operative, we are obliged to select a particular coordinate system and treat both of them on equal footing. Finally, one

should notice that the Kramers conjugation is also the unitary operation, since

$$\tilde{K}(\psi)K(\psi) = 1. \quad (29)$$

4. Velocity function in $Cl_{3,0}$

As we shall see in the future the velocity function is needed to establish correct boundary conditions in the interface between regions a and b . In the Hilbert space formulation the velocity operator is defined through the commutator in coordinate representation, or derivative in momentum representation:

$$\hat{v} = i[\hat{H}, \mathbf{x}] = \frac{\partial \hat{H}}{\partial \mathbf{p}}. \quad (30)$$

The conversion rules between Hilbert and Clifford algebra pictures [15] allow one to construct the following functions for x and y velocity components:

$$v_x(\psi) = \frac{\hbar k_x}{m^*}\psi + \frac{\alpha_D}{\hbar}\sigma_1\psi\sigma_3 - \frac{\alpha_R}{\hbar}\sigma_2\psi\sigma_3, \\ v_y(\psi) = \frac{\hbar k_y}{m^*}\psi + \frac{\alpha_R}{\hbar}\sigma_1\psi\sigma_3 - \frac{\alpha_D}{\hbar}\sigma_2\psi\sigma_3. \quad (31)$$

In coordinate representation the coordinates k_x and k_y must be replaced by $-i\partial/\partial x$ and $-i\partial/\partial y$. The above written velocity components do not commute. Indeed, one finds that the velocity commutator is

$$v_y(v_x(\psi)) - v_x(v_y(\psi)) = \frac{2}{\hbar^2}(\alpha_R^2 - \alpha_D^2)I\sigma_3\psi. \quad (32)$$

When $\alpha_R = \alpha_D$ the commutator vanishes. This special case, as noted in Ref. [28], is tolerant against spin-dependent scattering processes.

An average, i. e. physically measurable velocity, for example its x component $\langle v_x \rangle$, can be found from

$$\langle v_x \rangle = \tilde{\psi}v_x(\psi). \quad (33)$$

Elementary calculations give the following x components for $\psi_{a\pm}$ and $\psi_{b\pm}$ spinors

$$\langle v_{a\pm} \rangle = \frac{\hbar k_{a\pm}}{m_a^*} \pm \frac{\alpha_a}{\hbar}, \\ \langle v_{b\pm} \rangle = \frac{\hbar k_{b\pm}}{m_b^*} \pm \frac{\alpha_b}{\hbar}. \quad (34)$$

The wave vectors $k_{a\pm}$ and $k_{b\pm}$ are indicated in the Fig. 1. They are identified with spin-split energy subbands that are distinguished by opposite spin directions. The formulas (34) contain the standard velocity term

and plus/minus correction due to SO interaction. However, these formulas are awkward in analytical calculations because if they are applied the final results for reflection and transmission amplitudes are found to be very complicated and do not allow further simplification. Fortunately, the average velocity can be rewritten in a different form if instead of $k_{a\pm}$ and $k_{b\pm}$ the spin-degenerate band wave vectors, $k_a = \sqrt{2E_a m_a^*}$ and $k_b = \sqrt{2E_b m_b^*} = \sqrt{2(E_a - V) m_b^*}$, defined at energies E_a and E_b as shown in Fig 1, are used. Then one finds that

$$\begin{aligned} \langle v_{a\pm} \rangle &= \langle v_a \rangle = -\sqrt{(\hbar k_a / m_a^*)^2 + (\alpha_a / \hbar)^2}, \\ \langle v_{b\pm} \rangle &= \langle v_b \rangle = +\sqrt{(\hbar k_b / m_b^*)^2 + (\alpha_b / \hbar)^2}, \end{aligned} \quad (35)$$

where the signs before the square roots correspond to reflected and transmitted wave propagation direction. These equations explicitly demonstrate the important property that electron velocities in spin-split subbands (+) and (−) are equal if electron energy is fixed. This is not so evident from Eq. (34). Thus, the Eq. (35) implies that in all possible superposition states of ψ_+ and ψ_- the velocity will be the same and equal to (35) when electron energy is fixed, say, at the Fermi energy. By the same reason, in the following it is convenient to rewrite the spin-split wave vectors $k_{a\pm}$ and $k_{b\pm}$ in terms of degenerate band wave vectors, k_a and k_b , and SO coupling constants:

$$k_{a\pm} = \pm m_a^* \alpha_a / \hbar^2 - \sqrt{k_a^2 + (m_a^* \alpha_a / \hbar^2)^2}, \quad (36)$$

$$k_{b\pm} = \pm m_b^* \alpha_b / \hbar^2 - \sqrt{k_b^2 + (m_b^* \alpha_b / \hbar^2)^2}, \quad (37)$$

$$k_{i+} = +m_a^* \alpha_a / \hbar^2 + \sqrt{k_a^2 + (m_a^* \alpha_a / \hbar^2)^2}, \quad (38)$$

where (+) and (−) signs indicate respective eigenstates. The last line represents the wave vector for incident electronic beam in the region a .

5. Boundary conditions

When electron spin is neglected, the properties of boundary between two semiconductors is described by Ben-Daniel and Duke boundary condition which takes into account mass difference on both sides of the interface [29],

$$|\psi_a\rangle \Big|_{x=0^+} = |\psi_b\rangle \Big|_{x=0^-},$$

$$\frac{1}{m_a} \frac{\partial |\psi_a\rangle}{\partial x} \Big|_{x=0^+} = \frac{1}{m_b} \frac{\partial |\psi_b\rangle}{\partial x} \Big|_{x=0^-}. \quad (39)$$

In the presence of SO interaction the boundary conditions should be modified. When electron spin is included, the condition for continuity of spinor, now for Clifford spinor Ψ , remains valid,

$$\Psi_{a+} \Big|_{x=0^+} = \Psi_{b+} \Big|_{x=0^-}, \quad (40)$$

while the condition for derivative should be altered. To include the SO interaction in the derivative one has to start from an eight-band $\mathbf{k} \cdot \mathbf{p}$ model [30]. This line of reasoning was pursued by Pfeffer and Zawadzki [31, 32]. However the resulting formulas that follow from the multiple-band approach have been found too complex to be applicable for further analytical treatment of the problem. As indicated in references [33–35] the boundary conditions can be obtained in relatively simple way, by integrating the effective-mass Schrödinger equation across the interface $x = 0$. This results in the continuity condition for velocity

$$v_a(\Psi_{a+}) \Big|_{x=0^+} = v_b(\Psi_{b+}) \Big|_{x=0^-}, \quad (41)$$

where the velocity function is given by Eq. (31). The plus sign in the total spinor indicates that in (41) the incident wave is in ψ_+ state. Actually, one should demand the continuity of probability flux across the interface to be satisfied. Since the flux is the product of the probability density and velocity, while the spinor (and simultaneously the probability) is continuous at $x = 0$, instead of continuity of the derivative in (39) it is enough to require the continuity of the velocity. Thus, in the presence of SO interaction the multivector must satisfy conditions (40) and (41). In the following these conditions will be used to calculate the amplitudes of reflected and transmitted waves.

6. Total multivectors in regions a and b

As known, superposition of Hilbert space spinors multiplied by complex numbers also belongs to the same Hilbert space. Similar superposition can be constructed in the Clifford algebra. Since the latter is non-commutative, the superposition can be written in different forms, for example,

$$\begin{aligned} \Psi &= \psi_+ a + \psi_- b, \\ \Psi &= a \psi_+ + b \psi_- . \end{aligned} \quad (42)$$

So, the question arises which of the forms is correct and what is structure of the amplitudes a and b . The simplest

way to establish this is to address to conversion rule (11) between the Hilbert and Clifford algebra elements. In the case of the Hilbert space the coefficients a and b are complex numbers. Then, referring to the rule (11) one can write

$$\begin{aligned} a &= a_0 + a_3 I \sigma_3, \\ b &= b_0 + b_3 I \sigma_3, \end{aligned} \quad (43)$$

where a_0, a_3 , etc. are real. It can be verified that the square of the module of a general superposition Ψ then gives the correct form if the coefficients in the superposition are situated on the right-hand side of the spinors, i. e., we should have

$$\tilde{\Psi} \Psi = (\psi_+ a + \psi_- b) (\psi_+ a + \psi_- b) = a_0^2 + a_3^2 + b_0^2 + b_3^2, \quad (44)$$

where $\tilde{\Psi} = (\tilde{a} \tilde{\psi}_+ + \tilde{b} \tilde{\psi}_-)$. Since the composite spinor should be normalized, the coefficients should satisfy condition $a_0^2 + a_3^2 + b_0^2 + b_3^2 = 1$. As mentioned, in $Cl_{3,0}$ the spinor can be interpreted as a rotor while the Schrödinger equation may be treated as a dynamical equation for the rotor that controls the motion of classical (rather than quantum mechanical) spin [3, 36]. The interpretation of a in the superposition state can be seen from transformation

$$a \sigma_3 \tilde{a} = (a_0 + a_3 I \sigma_3) \sigma_3 (a_0 - a_3 I \sigma_3) = (a_0^2 + a_3^2) \sigma_3. \quad (45)$$

Thus the coefficients a and b change the length of vectors that are parallel to σ_3 . It can be shown that the vectors that are parallel to σ_1 and σ_2 , in addition, are rotated around σ_3 axis. From all what has been said we conclude that in a superposition state the multiplication of the ket vector $|\psi\rangle$ by complex amplitude A can be defined by rules

$$\begin{aligned} A &= a_0 + ia_3 \longleftrightarrow A = a_0 + a_3 I \sigma_3, \\ A|\psi\rangle &\longleftrightarrow \psi A, \end{aligned} \quad (46)$$

while in direction \mathbf{x} a running wave of amplitude A can be represented by multivector $\psi_{\pm} A e^{I \sigma_3 \mathbf{k} \cdot \mathbf{x}}$. Now we are prepared to construct the superposition of multivectors in regions a and b of the quantum well.

In the region $x < 0$ we have an incident wave in one of the eigenenergy subbands. For definiteness we shall assume that the incident wave of unit amplitude is in the eigenstate ψ_+ . After reflection from the discontinuity there appear two reflected waves having the same energy, the ordinary characterized by ψ_+ and the ex-

traordinary wave characterized by ψ_- . Thus, the total spinor in the region a is

$$\begin{aligned} \Psi_{a+} &= \psi_{a+} e^{I \sigma_3 \mathbf{k}_{a+} \cdot \mathbf{x}} + \psi_{a+} R_{++} e^{I \sigma_3 \mathbf{k}_{a+} \cdot \mathbf{x}} \\ &+ \psi_{a-} R_{+-} e^{I \sigma_3 \mathbf{k}_{a-} \cdot \mathbf{x}}. \end{aligned} \quad (47)$$

R_{++} and R_{+-} are the reflection amplitudes, where the first and second subscripts indicate the incident and reflected wave eigenstate respectively.

In the region b there are two transmitted waves

$$\Psi_{b+} = \psi_{b+} T_{++} e^{I \sigma_3 \mathbf{k}_{b+} \cdot \mathbf{x}} + \psi_{b-} T_{+-} e^{I \sigma_3 \mathbf{k}_{b-} \cdot \mathbf{x}}, \quad (48)$$

where T_{++} and T_{+-} are the transmission amplitudes. At $\mathbf{x} = 0$ the multivectors (47) and (48) in accordance with the boundary condition should be mutually equal.

If the incident wave is in ψ_- state, then in regions a and b the total spinors become

$$\begin{aligned} \Psi_{a-} &= \psi_{a-} e^{I \sigma_3 \mathbf{k}_{a-} \cdot \mathbf{x}} + \psi_{a-} R_{--} e^{I \sigma_3 \mathbf{k}_{a-} \cdot \mathbf{x}} \\ &+ \psi_{a+} R_{-+} e^{I \sigma_3 \mathbf{k}_{a+} \cdot \mathbf{x}}, \end{aligned} \quad (49)$$

$$\Psi_{b-} = \psi_{b-} T_{--} e^{I \sigma_3 \mathbf{k}_{b-} \cdot \mathbf{x}} + \psi_{b+} T_{-+} e^{I \sigma_3 \mathbf{k}_{b+} \cdot \mathbf{x}}. \quad (50)$$

R_{--} and R_{-+} are reflection, and T_{--} and T_{-+} are transmission amplitudes.

6.1. Amplitudes and their properties

After insertion of Ψ_{a+} and Ψ_{b+} into boundary conditions (40) and (41), and noting that in $Cl_{3,0}$ the momentum operator is replaced by

$$\hbar \hat{k}_x |\psi\rangle = -\hbar \frac{\partial |\psi\rangle}{\partial x} \longleftrightarrow -\hbar \frac{\partial \psi}{\partial x} I \sigma_3, \quad (51)$$

one obtains two algebraic multivector equations for unknown amplitudes. The simplest of these is the spinor continuity equation:

$$\psi_{a+} + \psi_{a+} R_{++} + \psi_{a-} R_{+-} = \psi_{b+} T_{++} + \psi_{b-} T_{+-}. \quad (52)$$

The continuity of the velocity is much more complex. For example, its right-hand side for the transmitted wave looks like

$$\begin{aligned} v_b(\Psi_{b+}) \Big|_{x=0} &= \frac{\hbar}{m_b^*} (k_{b+} \psi_{b+} T_{++} + k_{b-} \psi_{b-} T_{+-}) \\ &- \frac{1}{\hbar} (\alpha_{Db} \sigma_1 + \alpha_{Rb} \sigma_2) (\psi_{b+} T_{++} + \psi_{b-} T_{+-}) \sigma_3. \end{aligned} \quad (53)$$

Thus we have two multivector equations and four unknown amplitudes. One of the ways to solve such system is to resort to non-commutative Gröbner bases in

the Clifford algebras [37, 38]. However, we shall solve the system in a different way. The property that the multivector equation is equivalent to a system of 2^n real algebraic equations, where n is an order of the Clifford algebra, will be used. In our case $n = 3$. Thus, the boundary conditions yield the following system of coupled real linear equations for unknown amplitudes, where the coefficients at scalar and bivector parts of the amplitudes are supplied with superscripts (for example, $R_{++} = R'_{++} + R''_{++} I\sigma_3$):

$$R''_{++} + R''_{+-} - T''_{++} - T''_{+-} = 0, \quad (54)$$

$$1 + R'_{++} + R'_{+-} - T'_{++} - T'_{+-} = 0, \quad (55)$$

$$\begin{aligned} m_b^* \kappa_a (R''_{++} + R''_{+-}) \\ + m_a^* \kappa_b (T''_{++} + T''_{+-}) = 0, \end{aligned} \quad (56)$$

$$\begin{aligned} m_b^* \kappa_a (-1 + R'_{++} + R'_{+-}) \\ + m_a^* \kappa_b (T'_{++} + T'_{+-}) = 0, \end{aligned} \quad (57)$$

$$\begin{aligned} \alpha_b [\alpha_{Da} (1 + R'_{++} - R'_{+-}) \\ + \alpha_{Ra} (R''_{+-} - R''_{++})] \\ + \alpha_a [\alpha_{Db} (T'_{+-} - T'_{++}) \\ + \alpha_{Rb} (T''_{++} - T''_{+-})] = 0, \end{aligned} \quad (58)$$

$$\begin{aligned} \alpha_b [\alpha_{Ra} (1 + R'_{++} - R'_{+-}) \\ + \alpha_{Da} (R''_{++} - R''_{+-})] \\ + \alpha_a [\alpha_{Rb} (T'_{+-} - T'_{++}) \\ + \alpha_{Db} (T''_{+-} - T''_{++})] = 0, \end{aligned} \quad (59)$$

$$\begin{aligned} m_b^* \alpha_b \kappa_a [\alpha_{Da} (1 - R'_{++} + R'_{+-}) \\ + \alpha_{Ra} (R''_{++} - R''_{+-})] \\ + m_a^* \alpha_a \kappa_b [\alpha_{Db} (-T'_{++} + T'_{+-}) \\ + \alpha_{Rb} (T''_{++} - T''_{+-})] = 0, \end{aligned} \quad (60)$$

$$\begin{aligned} m_b^* \alpha_b \kappa_a [\alpha_{Ra} (1 - R'_{++} + R'_{+-}) \\ + \alpha_{Da} (-R''_{++} + R''_{+-})] \\ + m_a^* \alpha_a \kappa_b [\alpha_{Rb} (-T'_{++} + T'_{+-}) \\ + \alpha_{Db} (-T''_{++} + T''_{+-})] = 0, \end{aligned} \quad (61)$$

where effective wave vectors were introduced,

$$\begin{aligned} \kappa_a &= \sqrt{k_a^2 + (m_a^* \alpha_a / \hbar^2)^2}, \\ \kappa_b &= \sqrt{k_b^2 + (m_b^* \alpha_b / \hbar^2)^2}. \end{aligned} \quad (62)$$

In obtaining the above system we have used the formulas (36)–(38) that connect the wave vectors in degenerate and spin-split subbands. If instead of κ_a and κ_b one keeps nondegenerate wave vectors k_{a+} , k_{a-} , etc. shown by points in Fig. 1, the solution of the system (54)–(61), which can be found using a computer algebra package, appears very complicated and does not render further simplification. In addition, the interpretation of the solution is difficult.

In terms of effective wave vectors the system (54)–(61) gives the following very simple solution for reflection amplitudes of ordinary and extraordinary waves:

$$R_{++} = \frac{m_b^* \kappa_a - m_a^* \kappa_b}{m_b^* \kappa_a + m_a^* \kappa_b}, \quad R_{+-} = 0. \quad (63)$$

One sees that they have exactly the same form as reflection coefficient for zero-spin particle found in all textbooks on quantum mechanics. It should be noted that R_{++} is a scalar, i.e. $R_{++} = R'_{++}$. Since $R_{+-} = R'_{+-} + R''_{+-} I\sigma_3 = 0$, we conclude that the reflected wave has the same spin direction as the incident wave, however, the wavelength of the reflected wave is different as can be seen from k_{i+} and k_{a+} in Fig. 1.

The solution for a sum of transmitted amplitudes is real and resembles the textbook formula as well,

$$T_{++} + T_{+-} = \frac{2m_b^* \kappa_a}{m_b^* \kappa_a + m_a^* \kappa_b}. \quad (64)$$

However, the separate components in (64), apart from the scalar part, also contain the bivector part $I\sigma_3$:

$$\begin{aligned} T_{++} &= m_b^* \kappa_a [\alpha_a \alpha_b + \alpha_{Ra} \alpha_{Rb} + \alpha_{Da} \alpha_{Db} + I\sigma_3 \\ &\times (\alpha_{Ra} \alpha_{Db} - \alpha_{Rb} \alpha_{Da})] / [\alpha_a \alpha_b (m_b^* \kappa_a + m_a^* \kappa_b)], \end{aligned} \quad (65)$$

$$T_{+-} = m_b^* \kappa_a [\alpha_a \alpha_b - \alpha_{Ra} \alpha_{Rb} - \alpha_{Da} \alpha_{Db} - I\sigma_3$$

$$\times (\alpha_{Ra}\alpha_{Db} - \alpha_{Rb}\alpha_{Da}) \Big] / [\alpha_a\alpha_b(m_b^*\kappa_a + m_a^*\kappa_b)]. \quad (66)$$

It can be verified that the amplitudes (63)–(66) satisfy the probability continuity equation:

$$(1 + R_{++})^2 = |T_{++}|^2 + |T_{+-}|^2. \quad (67)$$

They also satisfy the current continuity equation

$$|\langle v_a \rangle| (1 - R_{++}^2) = |\langle v_b \rangle| (|T_{++}|^2 + |T_{+-}|^2), \quad (68)$$

where on the left-(right-)hand side of (68) stands the total flux in region a (b). The property (35) was used in obtaining the latter. From the continuity equations (67) and (68) the following approximate relation between the reflection coefficient and electron velocities in regions a and b can be obtained:

$$\left| \frac{\langle v_b \rangle}{\langle v_a \rangle} \right| = \frac{1 - R_{++}^2}{(1 + R_{++})^2} \approx 1 - |R_{++}|, \quad (69)$$

which may be useful in device construction.

Figure 2 shows the dependence of moduli of amplitudes of ordinary T_{++} and extraordinary T_{+-} transmitted waves as a function of Rashba coefficients in the regions a and b . The plots demonstrate that spin flipping is the largest when Rashba constants α_{Ra} and α_{Rb} have opposite signs. The probability of flipping is small or even vanishes at large Rashba constants having the same sign. Also, the plots demonstrate that the transition region from up to down spin occurs in the interval whose magnitude is of the order of Dresselhaus constant.

For a quantitative assessment of spin-flipping properties it is convenient to introduce experimentally measurable polarization parameter. Since the average velocities in spin-split subbands are equal (Eqs. (35)), the ratio of spin currents can be expressed through the transmission amplitudes. Therefore, the resulting spin current polarization magnitude can be defined by

$$P = \frac{|T_{++}|^2 - |T_{+-}|^2}{|T_{++}|^2 + |T_{+-}|^2}. \quad (70)$$

For the amplitudes (65) and (66) the polarization simplifies to a very elegant formula

$$P = \frac{\alpha_{Ra}\alpha_{Rb} + \alpha_{Da}\alpha_{Db}}{\sqrt{(\alpha_{Ra}^2 + \alpha_{Da}^2)(\alpha_{Rb}^2 + \alpha_{Db}^2)}}, \quad (71)$$

which depends on SO interaction constants of semiconductor only. We see that the outgoing beam will be depolarized totally when the product of SO constants satisfies the condition $\alpha_{Ra}\alpha_{Rb} + \alpha_{Da}\alpha_{Db} = 0$. On the

other hand, the transmitted beam will be totally polarized, $P = +1$ or $P = -1$, when one of the SO mechanisms vanishes, i. e. when either $\alpha_{Da} = \alpha_{Db} = 0$ or $\alpha_{Ra} = \alpha_{Rb} = 0$.

7. Summary and conclusions

We have formulated and solved general problem of spin flipping in terms of Clifford algebra $Cl_{3,0}$ when a two-dimensional electron is diffused by a stepped discontinuity in a quantum well. The discontinuity may include hetero- or homobarrier. A general boundary condition is presented which apart from mass difference also takes into account the difference in SO interaction constants on both sides of the discontinuity. It is shown that spin polarization of the transmitted beam can be

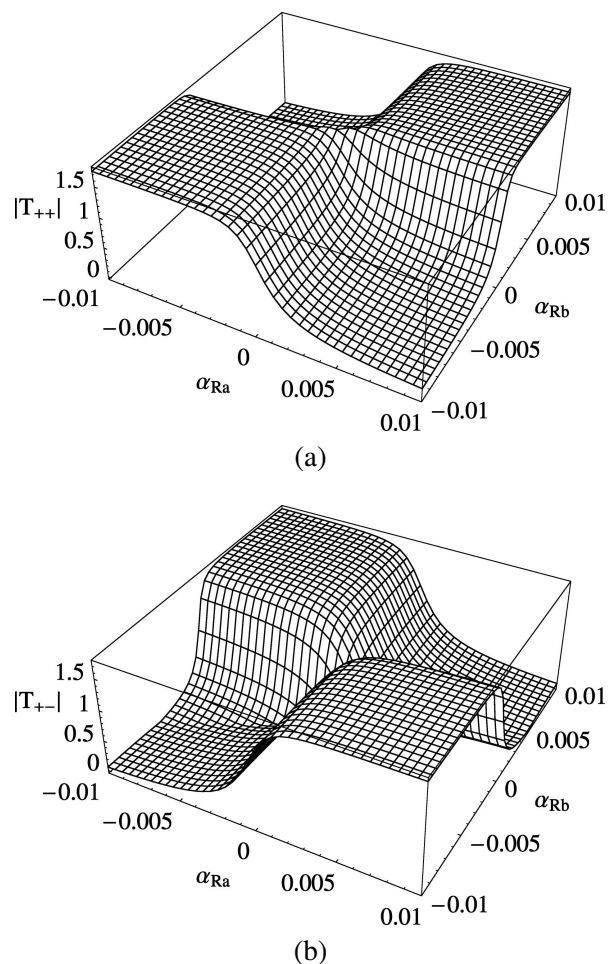


Fig. 2. Moduli of amplitudes of (a) ordinary and (b) extraordinary transmitted waves in Rashba coefficient plane marked in atomic units (a. u.). The incident wave is in state ψ_{a+} and has a well defined spin. The Rashba constants are varied in the range $\pm 1.44 \cdot 10^{-11}$ eV m = ± 0.01 a. u. The Dresselhaus constants have the following constant values: $\alpha_{Da} = 0.00139$ a. u. = $0.2 \cdot 10^{-11}$ eV m, $\alpha_{Db} = \alpha_{Da}/2$.

controlled by varying the SO interaction parameters. A general formula for polarization of the transmitted beam is presented. Depending on sign and values of the SO constants the transmitted electronic beam may be depolarized or its polarization may be inverted by a stepped discontinuity. Also the continuity equations that should be satisfied by the amplitudes of ordinary and extraordinary waves as well as electron velocities on both sides of discontinuity are presented. They may be useful in description of spin polarization in spintronic devices.

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DVIMAČIO ELEKTRONO SUKINIO VALDYMAS KVANTINIAME ŠULINYJE NAUDOJANT STAIGŲ FIZIKINIŲ PARAMETRŲ PASIKEITIMĄ

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Santrauka

Suformuluotas ir išnagrinėtas elektrono sukinio atspindžio ir pernašos uždavinys, kuriame atsižvelgta į staigų fizikinių parametrų pasikeitimą, pavyzdžiui, sukeliama sukinio ir orbitos sąveikos netolygumo, efektinių masių skirtumo arba potencialo laiptelio buvimo kvantiniame šulinyje. Uždavinys išspręstas pasitelkus Cliffordo algebras, dar vadinamos geometrine algebra, matematinę aparatą. Tiksliai išnagrinėtas atvejis, kai elektronas krinta statmenai netolygumo laipteliui. Parodyta, kad, nepaisant laiptelio savybių, atsispindėjusio elektroninio spindulio poliarizacija visada sutampa su krintančio spindulio poliarizacija. Tuo tarpu praėjusio pro ne-

tolygumą elektrono poliarizacija gali pasikeisti į priešingą. Nustatyta, kad bendruoju atveju praėjęs elektroninis spindulys sudarytas iš ordinarinės ir ekstraordinarinės bangų. Apibūdintos optimalios poliarizacijos apvertimo bei spindulio depoliarizacijos sąlygos, kurias turi atitikti kvantinio šulinio medžiaga abiejose parametrų trūkio pusėse. Gauta labai paprasta formulė, kurioje yra tik sukinio ir orbitos sąveikos konstantos ir kuri leidžia nustatyti praėjusio elektroninio spindulio poliarizaciją. Taip pat gautos elektrono spinoro amplitudės bei jo greičio nenutrūkstamumo lygtys, kurios gali praversti tuo atveju, kai elektrono sukinio judėjimas nagrinėjamas klasiškai.