Proceedings of the 14th International Symposium Ultrafast Phenomena in Semiconductors, Vilnius 2010

Double Reflection of Electron Spin in Semiconductors

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Reflection of spin-polarized electron from a potential barrier in bulk semiconductor in the presence of spin–orbit interaction is considered. The spin–orbit interaction brings about double electron reflection at oblique incidence of electronic beam onto the barrier. The competition between the Rashba and Dresselhaus spin–orbit mechanisms during double reflection is discussed. The problem was solved within the Clifford algebra framework, which allows one to describe the spin in a real Euclidean $\mathcal{E}_3$ space rather than in an abstract Hilbert space.

PACS: 85.75.−d, 72.25.Dc, 71.70.Ej, 03.65.Fd

1. Introduction

Recently it was shown that spin-polarized electron reflection off and transmission through a semitransparent barrier with spin–orbit (SO) interaction included is similar to polarized light behavior in a birefringent crystal [1–4]. In particular, in paper [4] it was shown that at oblique electron incidence the reflected beam in the quantum well is in a superposition of two beams having different wavelengths and reflection angles. This produces a two-period spatial spin beating pattern. Only Rashba SO interaction mechanism was taken into account. In this report the competition between the Rashba and Dresselhaus SO mechanisms in bulk cubic semiconductor during double spin reflection is discussed. The problem of spin reflection is formulated and solved within the Clifford algebra [5, 6] framework. In the second section the Hamiltonian is considered. The results on spin reflection are presented in the third section.

2. Hamiltonian and eigenbivectors

The Schrödinger equation for conduction band electron in a cubic semiconductor, when the SO interaction is included, has the following compact form after its transformation to $Cl_{3,0}$ noncommutative Clifford algebra [4, 6, 7],

$$\frac{\partial\psi}{\partial t} I\boldsymbol{\sigma}_3 = \varepsilon_0\psi + \boldsymbol{\varepsilon}\psi\boldsymbol{\sigma}_3\,. \tag{1}$$

Here $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ are basis vectors and $I = \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\boldsymbol{\sigma}_3$ is the pseudoscalar. The basis vectors are isomorphic to the Pauli matrices and satisfy $\boldsymbol{\sigma}_i^2 = 1$, $\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j\boldsymbol{\sigma}_i = 0$. In the following the bivectors $I\boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_2\boldsymbol{\sigma}_3$, $I\boldsymbol{\sigma}_2 = \boldsymbol{\sigma}_3\boldsymbol{\sigma}_1$ and $I\boldsymbol{\sigma}_3 = \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2$, which represent the orientated planes, will be used, too. The right-hand side of (1) may be thought of as a Hamiltonian function of the multivector ψ (analogue of the spinor in the traditional formulation),

$$H(\psi) = \varepsilon_0\psi + \boldsymbol{\varepsilon}\psi\boldsymbol{\sigma}_3\,. \tag{2}$$

Equation (1) has an invariant form with the quantization axis parallel to direction $\boldsymbol{\sigma}_3$. The scalar ε_0 describes the degenerate conduction band spectrum

$$\varepsilon_0 = \boldsymbol{k}\cdot\boldsymbol{k}/2m^* = \left(k_1^2 + k_2^2 + k_3^2\right)/2m^*, \tag{3}$$

where k_i's are the components of electron wave vector $\boldsymbol{k} = k_1\boldsymbol{\sigma}_1 + k_2\boldsymbol{\sigma}_2 + k_3\boldsymbol{\sigma}_3$ and m^* is the effective mass. The inner product of vectors is indicated by dot in (3). As we shall see the vector $\boldsymbol{\varepsilon}$ in (1) is parallel to quantum mechanical average spin of electron. When $\boldsymbol{\sigma}_i$'s are aligned with the cubic crystal axes the vector $\boldsymbol{\varepsilon}$ can be expanded in components

$$\boldsymbol{\varepsilon} = \varepsilon_1\boldsymbol{\sigma}_1 + \varepsilon_2\boldsymbol{\sigma}_2 + \varepsilon_3\boldsymbol{\sigma}_3\,. \tag{4}$$

The projections ε_i (scalars) in the presence of the Dresselhaus and Rashba SO interaction are

$$\varepsilon_1 = \gamma_{\rm D}k_1\left(k_2^2 - k_3^2\right) + \alpha_{\rm R}\left(k_2n_3 - k_3n_2\right) \quad \text{and cycl. perm.} \tag{5}$$

Here $\alpha_{\rm R}$ and $\gamma_{\rm D}$ are the Rashba and Dresselhaus constants. In (5), the projections ε_i are expressed through the wave vector $\boldsymbol{k}$ and unit vector $\boldsymbol{n} = n_1\boldsymbol{\sigma}_1 + n_2\boldsymbol{\sigma}_2 + n_3\boldsymbol{\sigma}_3$ normal to the Rashba plane. The vector $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{\rm R} + \boldsymbol{\varepsilon}_{\rm D}$ can be rewritten in an invariant form, too. The Rashba term has the following coordinate-independent shape

$$\boldsymbol{\varepsilon}_{\rm R} = \alpha_{\rm R}I\boldsymbol{n}\wedge\boldsymbol{k}\,, \tag{6}$$

where the wedge represents the outer product of two vectors: $\boldsymbol{a}\wedge\boldsymbol{b} = (\boldsymbol{ab} - \boldsymbol{ba})/2$. For the Dresselhaus SO interaction the respective term is

$$\boldsymbol{\varepsilon}_{\rm D} = -\frac{\gamma_{\rm D}}{2}\left[(\boldsymbol{k}_{12}\boldsymbol{\sigma}_1)^2 + (\boldsymbol{k}_{23}\boldsymbol{\sigma}_2)^2 + (\boldsymbol{k}_{31}\boldsymbol{\sigma}_3)^2\right]\boldsymbol{k} - 3\gamma_{\rm D}(\boldsymbol{k}\cdot\boldsymbol{\sigma}_1)(\boldsymbol{k}\cdot\boldsymbol{\sigma}_2)(\boldsymbol{k}\cdot\boldsymbol{\sigma}_3)I\,, \tag{7}$$

where the vectors $\boldsymbol{k}_{ij}$ lie in the orthogonal planes indicated by subscripts, $\boldsymbol{k}_{12} = (\boldsymbol{k} - \boldsymbol{\sigma}_3\boldsymbol{k}\boldsymbol{\sigma}_3)/2$ and cycl. perm. It should be noted that contrary to the Rashba

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contribution (6) here the basis vectors $\boldsymbol{\sigma}_1$, $\boldsymbol{\sigma}_2$ and $\boldsymbol{\sigma}_3$ cannot be eliminated altogether, since we must somehow indicate the cubic crystal axes with respect to which the Dresselhaus Hamiltonian has been written.

The solution of the multivector Schrödinger Eq. (1) is**

$$\psi(t) = \psi_{\rm i}\psi_{\varepsilon}\psi_{\varepsilon_0} = \psi_{\rm i}\,{\rm e}^{-I\boldsymbol{\varepsilon}t}\,{\rm e}^{-\varepsilon_0 I\boldsymbol{\sigma}_3 t}, \tag{8}$$

where $\psi_{\rm i}$ is the initial multivector at the moment $t = 0$ which satisfies the normalization condition $\tilde{\psi}_{\rm i}\psi_{\rm i} = 1$, where the tilde denotes the reversion [6]. Equation (8) describes the beating in spin-split band at average electron energy $\varepsilon_0 + \varepsilon_3$. In the Clifford algebra $Cl_{3,0}$ the average of a multivector function $O(\psi)$ is $\langle O\rangle = \langle\tilde{\psi}O(\psi)\rangle - \langle\tilde{\psi}O(\psi)I\boldsymbol{\sigma}_3\rangle I\boldsymbol{\sigma}_3$, where the brackets denote the scalar part [6]. The second term proportional to the bivector $I\boldsymbol{\sigma}_3$ usually is equal to zero [6]. Then, after the insertion of time-dependent solution (8) one gets the following average energy: $\langle\varepsilon\rangle = \langle\tilde{\psi}H(\psi)\rangle = \varepsilon_0 + \varepsilon_3$. This energy is different from spin-split subband eigenenergies ε_+ and ε_-. In terms of ε_0 and $\boldsymbol{\varepsilon}$ the latter are [7]:

$$\varepsilon_\pm = \varepsilon_0 \pm \sqrt{\boldsymbol{\varepsilon}\cdot\tilde{\boldsymbol{\varepsilon}}} = \varepsilon_0 \pm \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2}\,, \tag{9}$$

where the quantity $\varepsilon = \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2}$ represents the spin splitting energy $\Delta\varepsilon = 2\varepsilon$. This shows that the solution (8) represents a superposition of the up and down spin states.

In the analysis of spin reflection we shall need the eigenbivectors $\psi_\pm$ (analogues of eigenfunctions) which must satisfy the eigenbivector equation

$$H(\psi_\pm) = \varepsilon_\pm\psi_\pm\,, \tag{10}$$

where the Hamiltonian function is represented by (2). Multiplying both sides of (10) by $\tilde{\psi}$ one can write $\tilde{\psi}_\pm H(\psi_\pm) = \varepsilon_\pm$, where the left and right hand sides now are scalars. Insertion of a general quaternion $\psi = c_0 + c_1 I\boldsymbol{\sigma}_1 + c_2 I\boldsymbol{\sigma}_2 + c_3 I\boldsymbol{\sigma}_3$, where c_i's are unknown scalars, gives a system of equations that can be solved with respect to scalars c_i's. This gives the following eigenbivectors:

$$\psi_\pm = -\frac{I(\boldsymbol{\varepsilon} \pm \varepsilon\boldsymbol{\sigma}_3)}{\sqrt{2\varepsilon(\varepsilon \pm \varepsilon_3)}}\,. \tag{11}$$

They are normalized: $\tilde{\psi}_+\psi_+ = 1$ and $\tilde{\psi}_-\psi_- = 1$. The property $\boldsymbol{\varepsilon}^2 = \varepsilon^2 = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2$ was used in obtaining (11). From the latter expression one sees that the products $I\psi_+$ and $I\psi_-$ represent two vectors which can be obtained from the spin vector $\boldsymbol{\varepsilon}$ by adding the vectors $\pm\varepsilon\boldsymbol{\sigma}_3$. The denominator in (11) is nothing else than the normalization constant.

The average spin vector $\boldsymbol{s}$ in the Clifford algebra is determined by geometric product $\boldsymbol{s} = \psi\boldsymbol{\sigma}_3\tilde{\psi}$ [6]. Using the above eigenbivectors we can find that the average spin vector for conduction band electron is

$$\boldsymbol{s}_\pm = \psi_\pm\boldsymbol{\sigma}_3\tilde{\psi}_\pm = \pm\boldsymbol{\varepsilon}/\varepsilon\,, \tag{12}$$

which shows that the vector $\boldsymbol{\varepsilon}$ in the Hamiltonian function (2) is indeed linked with the average spin direction. This is true for a general case independent of SO interaction type. Also, one can show that for an arbitrary SO interaction the spin vector is not perpendicular to the wave vector, since the product $\boldsymbol{k}\cdot\boldsymbol{s} \neq 0$. However, in the presence of the Rashba SO interaction only, when $\gamma_{\rm D} = 0$ in (5), one can show that $\boldsymbol{k}\cdot\boldsymbol{s} = 0$, in agreement with the standard calculations in the Hilbert space.

3. Spin reflection from (100) barrier

We shall consider a beam of ballistic electrons that bounce off an infinite barrier at $x = 0$, as shown in Fig. 1. Here the basis vector $(\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)$ directions can be identified with x, y and z axes. The total spinor (multivector) $\Psi_+(x, y)$ in the region $x > 0$ consists of the sum of quaternions that describe the incident wave $\boldsymbol{k}_{\rm i+}$ at angle γ and the reflected waves $\boldsymbol{k}_{\rm r+}$ and $\boldsymbol{k}_{\rm r-}$ at angles α and β, respectively,

$$\Psi_+(x, y) = \psi_+(\gamma)A_{\rm i+}\,{\rm e}^{I\boldsymbol{\sigma}_3\boldsymbol{k}_{\rm i+}\cdot\boldsymbol{r}} + \psi_+(\beta)A_{\rm r+}\,{\rm e}^{I\boldsymbol{\sigma}_3\boldsymbol{k}_{\rm r+}\cdot\boldsymbol{r}} + \psi_-(\alpha)A_{\rm r-}\,{\rm e}^{I\boldsymbol{\sigma}_3\boldsymbol{k}_{\rm r-}\cdot\boldsymbol{r}},$$

where $\psi_\pm$ are eigenquaternions (11) and $A_{\rm i}$'s are unknown amplitudes (multivectors). For an infinite barrier the boundary condition $\Psi_+(0, y) = 0$ should be satisfied. Similar equation can be written for spinor $\Psi_-(x, y)$ when the incident wave lies on ε_- surface. When both the Rashba and Dresselhaus mechanisms are included the constant energy surfaces are rather complicated. By this reason here we shall consider only symmetric case (compare Fig. 1) when the barrier lies in (100)-type plane.

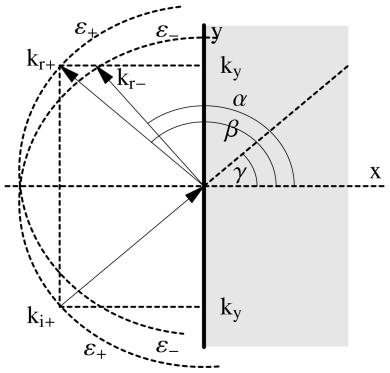

Fig. 1. Spin dependent reflection of electron having the incident wave vector $\boldsymbol{k}_{\rm i+}$ on ε_+ surface. $\boldsymbol{k}_{\rm r+}$ and $\boldsymbol{k}_{\rm r-}$ are the wave vectors of reflected waves having opposite spin states. The dashed circles represent constant energy surfaces $\varepsilon_+ = \varepsilon_-$ in $\boldsymbol{k}$-space. Since the component k_y is conserved during scattering process, one has $\beta + \gamma = \pi$ in this case.

** Here we shall take a chance to amend formulae (12) and (13) in [7]. The correct ones are given, respectively, by (1) and (8) in the present paper. This has no influence on subsequent material of Ref. [7].

3.1. Dresselhaus SO interaction

When $\alpha_{\rm D} \neq 0$ and $\alpha_{\rm R} = 0$, the eigenbivectors (11) become independent of material parameters. The reflection amplitudes $|R_{++}|^2$ and $|R_{+-}|^2$ then appear to be independent of material parameters, too. The first and second subscripts in R indicate the ingoing and outgoing waves, respectively. Solid lines in Fig. 2a show the reflection coefficients $|R_{++}|^2$ and $|R_{+-}|^2$ as a function of x-projection k_{xi+} of the incident electron wave vector $\boldsymbol{k}_{\rm i+}$. The figure shows that at nearly vertical incidence, when $k_y \approx 0$ and k_{xi+} is the largest, the extraordinary wave characterized by $|R_{+-}|^2$ does not appear. At the grazing incidence, when $k_{xi+} \approx 0$, nearly all electronic wave transforms to extraordinary wave. Similar behavior is found when the ingoing wave is on ε_- surface, as shown by solid lines in Fig. 2b.

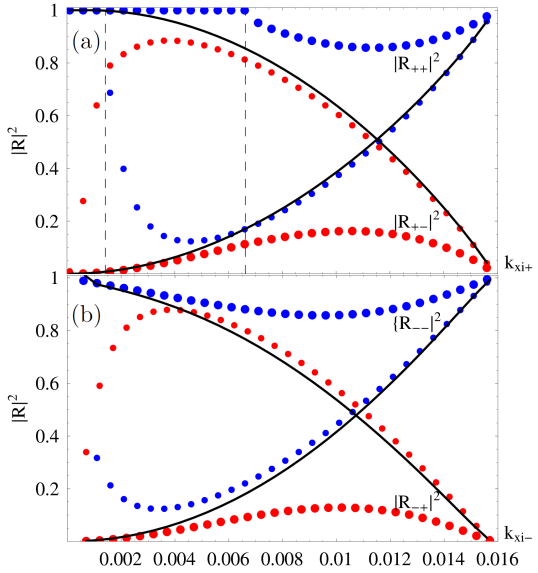

Fig. 2. Squared moduli of reflection coefficients vs. incident electron wave vector component perpendicular to barrier. The wave vector is in atomic units, 1 a.u. = 18.89 nm^{-1}. For all curves $\gamma_{\rm D} = 100$ eV Å^3. Solid lines — $\alpha_{\rm R} = 0$. Small dots — the Dresselhaus contribution predominates, $\alpha_{\rm R} = 0.0057$ eV Å. Large dots — the Rashba contribution predominates, $\alpha_{\rm R} = 0.1007$ eV Å. (a) Incident electron wave vector end lies on $\varepsilon_+ = 34$ meV surface; the vertical dashed lines show critical values of k_{xi+} component. (b) Incident electron wave vector end lies on $\varepsilon_- = 34$ meV surface.

3.2. Rashba SO interaction

When $\gamma_{\rm R} \neq 0$ and $\gamma_{\rm D} = 0$ we find that independently of the incidence angle no superposition between spin-split states takes place in this case at all. Only ordinary reflected waves are present. Before and after reflection the average spin lies in x–y plane and always remains perpendicular to $\boldsymbol{k}$.

3.3. Rashba+Dresselhaus SO interaction

The points in Fig. 2 show the results of numerical calculations. The small points correspond to relatively weak influence of the Rashba interaction, $\alpha_{\rm R} = 0.0057$ eV Å, while the large points correspond to interaction where the Rashba contribution predominates, $\alpha_{\rm R} = 0.1007$ eV Å. The other parameters were $m^* = 0.1\,m_0$, $\gamma_{\rm D} = 100$ eV Å^3, the Fermi energy $\varepsilon_{\rm F} = 34$ meV. When the projections k_{xi+} and k_{xi-} of the incident wave are large (this corresponds to nearly normal incidence, $k_y \approx 0$) we observe the extraordinary reflected beam whose polarization is opposite to incident one. However, at grazing incidence, when the projections k_{xi+} and k_{xi-} are small, one observes strong competition between the Rashba and Dresselhaus mechanisms. If $\gamma \to \pi/2$, the Dresselhaus mechanism vanishes and the contribution of the Rashba mechanism in the dispersion always becomes predominant, as a result one observes a violent switching from one to the other mechanism at small k_{xi+} and k_{xi-} values.

The vertical dashed lines in Fig. 2a show the critical values for the total reflection of extraordinary waves, the origin of which can be traced from Fig. 1. There is no critical angle when the ingoing electron wave vector end lies on ε_- surface. As shown in [4] the interference between ordinary and extraordinary reflected waves gives double-period spatial beating pattern in wave function amplitude and spin components. Similar spin beating was found in the present case.

4. Conclusions

In conclusion, it is shown that in bulk semiconductors in the presence of SO interaction and under an oblique incidence the electron reflection from the barrier occurs at two different angles which gives superpositions of states having opposite spins and, consequently, spatial spin beating between incident and two reflected waves.

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