Lithuanian Journal of Physics, Vol. **46**, No. 1, pp. 27–31 (2006)

FREE ELECTRON SPIN IN CUBIC SEMICONDUCTORS

A. Dargys

Semiconductor Physics Institute, A. Goštauto 11, LT-01108 Vilnius, Lithuania
E-mail: dargys@pfi.lt

Received 4 November 2005

The spin surface describes all possible spin states, including superposition states, of a free charge carrier in a particular energy band. Due to a finite spin–orbit interaction in semiconductors, the spin surface normally has a form of the spheroid, the orientation of which depends on the carrier wave vector direction. The paper shows that in cubic semiconductors the spin surface of the conduction band electron has spherical shape, despite the nonsphericity of the constant energy surface induced by a finite spin–orbit interaction. Also, it is shown that this property is universal, i. e., it is independent of the electron wave vector direction and energy band parameters.

Keywords: spintronics, electron spin, semiconductors

PACS: 85.75.-d, 72.25.Rb, 67.57.Lm

1. Introduction

Calculations of the spin-related properties in semiconductor heterostructures usually proceeds in two stages. In the first, bulk (3D) spinors are constructed in the respective homogeneous regions of the heterostructure and then, in the second stage, the corresponding boundary conditions are imposed on the bulk spinors at interfaces between constituent materials of the heterostructure, what allows one to find the resulting spinor in the 2D heterostructure. In 3D semiconductors, the conduction band spin is taken into account by Dresselhaus and Rashba Hamiltonians that include a finite spin–orbit interaction in the semiconductor lattice. Because the Hamiltonians are relativistic by their origin, the total Hamiltonian normally does not commute with the spin operator and the spin surface that describes all possible eigenspin superpositions in the spin space does not possess spherical symmetry. Normally it has the form of the spheroid (ellipsoid of rotation). The orientation of the spheroid is determined by charge carrier wave vector $\mathbf{k}$. Since the spin–orbit interaction is a relativistic effect, the spin formally should be characterized by the helicity quantum number. In this note we shall show that despite relativistic ingredients in the origin of the conduction band Hamiltonian the electron spin surfaces in A_3B_5 and A_2B_6 compounds remain spherical for both the Dresselhaus and Rashba Hamiltonians, as well as for the combined Hamiltonian, independent of the direction of $\mathbf{k}$ and the conduction band parameters. From this it follows that the spin quantization axis can be chosen to point to an arbitrary, not necessarily related with the crystallographic axes direction in solving the problems related with the conduction band spin in cubic semiconductors and heterostructures, where the spatial quantization is important.

2. Hamiltonians

Conduction band minimum in cubic A_3B_5 and A_2B_6 semiconductors is located at the centre of the Brillouin zone. At not too large energies, the dispersion in the vicinity of the minimum is proportional to the square of the electron wave vector $\mathbf{k}$ and coincides with that of a nonrelativistic free electron,

$$H_0 = \frac{\mathbf{k}^2}{2m^*}\,\mathbb{I}\,. \tag{1}$$

However, instead of the free electronic mass m_0, the effective mass m^* appears in the dispersion (1). Usually, one has that $m^* < m_0$. Atomic units are used in this paper: $m_0 = e = \hbar = 1$. Thus, m^* is dimensionless. The 2×2 unit matrix $\mathbb{I}$ in (1) indicates that the electron may be in two, up and down spin eigenstates with respect to some arbitrarily chosen spin quantization axis. The Hamiltonian (1), in fact, does not represent true spin properties of a free electron in a semiconductor and merely states that the conduction band

ISSN 1648-8504

electron possesses only two spin eigenstates. If statistical properties of the electrons are important only, the matrix $\mathbb{I}$ doubles the density of states. Two types of spin-related Hamiltonians that, due to spin–orbit interaction, take into account the splitting of the conduction band Hamiltonian (1) are known at present. The first, Dresselhaus Hamiltonian [1], is related with the inversion asymmetry of the microscopic crystal potential of the otherwise homogeneous semiconductor, and the second, Rashba Hamiltonian [2], is related with the structural inversion asymmetry, or asymmetry of the confining potential in 2D heterostructures, for example due to the presence of the interface.

The Dresselhaus Hamiltonian can be constructed from crystal lattice symmetry considerations with the spin–orbit interaction included in the lattice periodic Hamiltonian [1]. In the Dresselhaus Hamiltonian, the spin-splitting of the conduction band is described by terms that are cubic in the wave vector. In a short form the Hamiltonian is

$$H_{\rm D} = \gamma\, \boldsymbol{\sigma} \cdot \boldsymbol{\chi}, \tag{2}$$

where the proportionality constant γ, or Dresselhaus constant, determines the strength of the spin splitting of the doubly degenerate energy band. The vector $\boldsymbol{\chi} = (\chi_x, \chi_y, \chi_z)$ is proportional to cube of the wave vector components, $\mathbf{k} = (k_x, k_y, k_z)$, for example, $\chi_x = k_x(k_y^2 - k_z^2)$. The other components of $\boldsymbol{\chi}$ can be found by cyclic permutation of the respective Cartesian wave vector components. In (2), $\boldsymbol{\sigma}$ is the vector consisting of the Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. It should be stressed that k_i's are referenced with respect to crystallographic axes of the material and the Hamiltonian (2) is written in the σ_z representation, where the electron spin quantization axis is parallel to $[001]$ crystallographic axis.

As mentioned, the Rashba Hamiltonian is related with the structural inversion asymmetry, which takes into account the spin splitting due to, for example, presence of a heterojunction or a quantum well in the bulk of the semiconductor. A critical review on the properties of this Hamiltonian was recently given in Ref. [3]. The Rashba Hamiltonian is proportional to the first power of the wave vector,

$$H_{\rm R} = \alpha\, (\boldsymbol{\sigma} \times \mathbf{k}) \cdot \boldsymbol{\nu}, \tag{3}$$

where $\boldsymbol{\nu}$ is the unit vector parallel to heterostructure growth direction (usually it is normal to k_x–k_y plane) and α is the coupling (Rashba) constant. When $\boldsymbol{\nu}$ is perpendicular to (001) plane, in the cylindrical coordinate system where $k_x = k_{||}\cos\varphi$, $k_y = k_{||}\sin\varphi$, the Rashba Hamiltonian assumes the following form:

$$H_{\rm R} = \alpha k_{||} \begin{bmatrix} 0 & {\rm i}{\rm e}^{-{\rm i}\varphi} \\ -{\rm i}{\rm e}^{{\rm i}\varphi} & 0 \end{bmatrix}. \tag{4}$$

The total conduction band Hamiltonian, the spin properties of which interest us, consists of the sum of all the three above discussed Hamiltonians:

$$H = H_0 + H_{\rm D} + H_{\rm R}\,. \tag{5}$$

In the expanded form, in the up $|\uparrow\rangle$ and down $|\downarrow\rangle$ spin basis with the quantization axis parallel to k_z, the Hamiltonian (5) is a 2×2 matrix:

$$H = \tag{6}$$

$$\begin{bmatrix} E_0 + \gamma\chi_z & {\rm i}\alpha k_{||}{\rm e}^{-{\rm i}\varphi} + \gamma(\chi_x - {\rm i}\chi_y) \\ -{\rm i}\alpha k_{||}{\rm e}^{{\rm i}\varphi} + \gamma(\chi_x + {\rm i}\chi_y) & E_0 - \gamma\chi_z \end{bmatrix},$$

where $E_0 = \mathbf{k}^2/(2m^*)$. Since the Rashba Hamiltonian possesses the lowest symmetry, the total Hamiltonian derives its symmetry properties from the Rashba Hamiltonian, namely, the D_{2d} symmetry of the point group.

The two eigenvalues E_1 and E_2 (dispersion laws) of the total Hamiltonian (6) describe the energies of the conduction band as a function of electron wave vector. Simple calculations using (6) give

$$E_{1,2} = E_0 \pm \xi = \tag{7}$$

$$E_0 \pm \sqrt{\alpha^2 k_{||}^2 + \gamma^2 \boldsymbol{\chi}^2 + 2\alpha\gamma k_{||}(\chi_x \sin\varphi - \chi_y \cos\varphi)}\,.$$

The largest contribution in the dispersion (7) comes from the first (spherical) term. The second term describes the spin splitting in the conduction band, $\Delta E = E_2 - E_1 = 2\xi$. The last term under the square root shows that the mixing of Dresselhaus and Rashba mechanisms takes place, and the splitting cannot be represented as separate contributions of individual Dresselhaus and Rashba mechanisms. Figure 1 shows the character of constant energy surfaces calculated with (7), where band parameters of GaAs were used, but with α and γ values increased to emphasize the differences between the two surfaces. In real semiconductors the splitting is small (about 1 meV) and, therefore, in standard analysis of optical or transport properties it is often neglected. However, in the analysis of electron spin properties the inclusion of both energy bands is of principal importance.

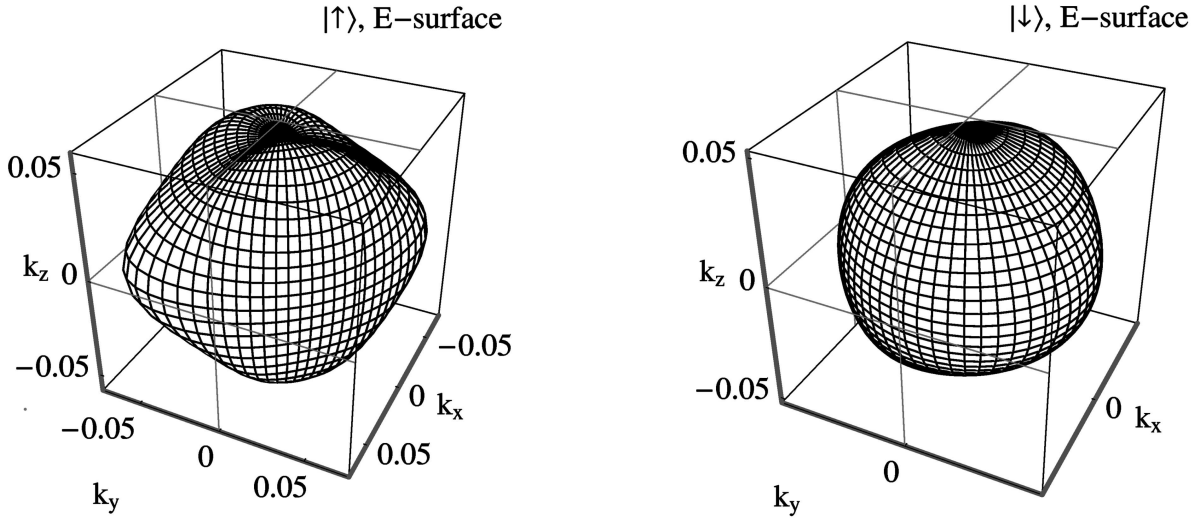

Fig. 1. Constant energy surfaces of the spin-split conduction bands calculated at energy $E = 0.5$ eV. The (a) left and (b) right surfaces correspond to minus and plus signs in Eq. (7). In real semiconductors the energy band warping is smaller and, therefore, the shape of the surfaces is much closer to spherical.

3. Spin surface

The quantum mechanics teaches that two physical quantities can be measured simultaneously (in the sense of eigenvalues) if their respective operators commute. In our case the commutator of the spin operator $\mathbf{S} = \boldsymbol{\sigma}/2$ with the total Hamiltonian (5) does not reduce to zero matrix. For example, the commutator with the S_z component gives

$$[H, S_z] = \tag{8}$$

$$\begin{bmatrix} 0 & -\mathrm{i}\alpha k_{||}\mathrm{e}^{-\mathrm{i}\varphi} - \gamma(\chi_x - \mathrm{i}\chi_y) \\ -\mathrm{i}\alpha k_{||}\mathrm{e}^{\mathrm{i}\varphi} + \gamma(\chi_x + \mathrm{i}\chi_y) & 0 \end{bmatrix}.$$

The other commutators, $[H, S_x]$ and $[H, S_y]$, are not equal zero as well, except the trivial case when $\mathbf{k} = 0$. From this follows that the energy and spin projections cannot be good quantum numbers simultaneously. Thus, one expects that, due to noncommutivity, the spin surface is not of spherical shape, or deviates from the sphericity insignificantly if the spin splitting energy ΔE is small. In case of the valence band holes the deviation is very large, as shown in Refs. [4–7].

In the analysis and interpretation of physical properties in semiconductors it is a common practice to use the energy band representation, where the electron is described by a well-defined energy and wave vector. Thus, in the following instead of the eigenvalues of the spin operator $\mathbf{S} = \boldsymbol{\sigma}/2$ we shall be concerned with the quantum mechanical average spin $\langle \mathbf{S} \rangle$. In Refs. [4–7] it has been shown that in such case in the analysis of spin properties of a free, ballistic hole it is better to think in terms of a spin surface in the spin space. The latter determines all possible spin directions and magnitudes of a free charge carrier that propagates with a given wave vector $\mathbf{k}$ in one of the allowed energy bands. Mathematically the spin surface represents all possible realizations of the average spin,

$$\langle \mathbf{S} \rangle = (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle)/2, \tag{9}$$

where $\langle \sigma_i \rangle = \langle \psi | \sigma_i | \psi \rangle$. The spinor $|\psi\rangle$ represents all possible superpositions of up and down spin eigenstates. The simplest way to construct $|\psi\rangle$ is to switch over to the energy band representation and then parametrize the spinor, for example, in the following form:

$$|\vartheta, \phi\rangle = \begin{bmatrix} \sin\vartheta \\ \cos\vartheta \mathrm{e}^{\mathrm{i}\phi} \end{bmatrix}. \tag{10}$$

To connect the spinor (10) with its counterpart $|\psi\rangle$ in the σ_z representation one must know the unitary transformation matrix U that connects both representations. Then the both spinors can be linked by

$$|\vartheta, \phi\rangle = U|\psi\rangle\,. \tag{11}$$

The simplest way to find U is to calculate the eigenvectors of the Hamiltonian (5) and using the eigenvectors

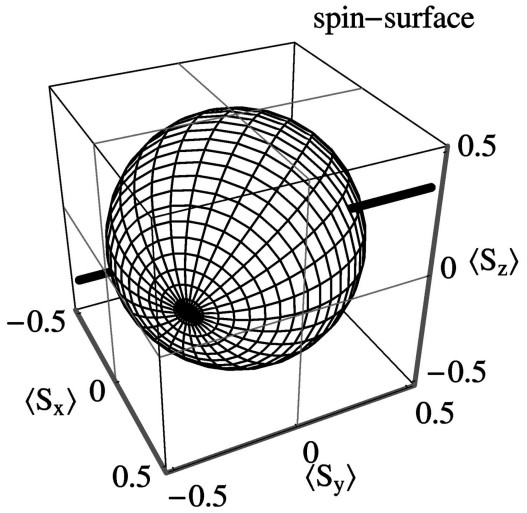

Fig. 2. Spin surface of the free electron in A_3B_5 and A_2B_6 semiconductors. In this case the poles on the sphere lie on the spin quantization axis. The thick line shows the direction of the wave vector $\mathbf{k} = (k_{||}, \varphi, k_z)$. $k_{||} = 0.1$ a.u., $k_z = 0.05$ a.u., $\varphi = \pi/4$.

to construct an appropriate 2×2 matrix. The orthonormalized eigenvectors of (5) are

$$\mathbf{v}_1 = \begin{bmatrix} -\dfrac{\mathrm{i}(\xi - \gamma\chi_z)}{\sqrt{\zeta^2 + (\xi - \gamma\chi_z)^2}} \\ \dfrac{\mathrm{e}^{\mathrm{i}\varphi}\alpha k_{||} + \gamma(\mathrm{i}\chi_x - \chi_y)}{\sqrt{\zeta^2 + (\xi - \gamma\chi_z)^2}} \end{bmatrix}, \qquad (12)$$

$$\mathbf{v}_2 = \begin{bmatrix} \dfrac{\mathrm{i}(\xi + \gamma\chi_z)}{\sqrt{\zeta^2 + (\xi + \gamma\chi_z)^2}} \\ \dfrac{\mathrm{e}^{\mathrm{i}\varphi}\alpha k_{||} + \gamma(\mathrm{i}\chi_x - \chi_y)}{\sqrt{\zeta^2 + (\xi + \gamma\chi_z)^2}} \end{bmatrix}, \qquad (13)$$

where ζ is defined by $\zeta^2 = \alpha^2 k_{||}^2 + \gamma^2(\chi_x^2 + \chi_y^2) + 2\alpha\gamma k_{||}(\chi_x \sin\varphi - \chi_y \cos\varphi)$ and ξ has been given earlier in Eq. (7). If $k_z = 0$, then $\xi_{k_z=0} = \zeta$. The knowledge of the eigenvectors allows one to form the unitary transformation matrix that brings the Hamiltonian to the diagonal form [8]. The required matrix is $U = (\mathbf{v}_1^*, \mathbf{v}_2^*)$, where $\mathbf{v}_1^*$ and $\mathbf{v}_2^*$ are to be understood, respectively, as the first and the second row of the matrix U. Then, with the help of U the total Hamiltonian (5) diagonalizes to

$$UHU^\dagger = \begin{pmatrix} E_0 - \xi & 0 \\ 0 & E_0 + \xi \end{pmatrix}. \qquad (14)$$

Of course, the same unitary transformation matrix U can be used to bring the parametrized spinor (10) to the initial σ_z representation, where using the Pauli matrices the components $\langle S_i \rangle = \langle \psi | \sigma_i | \psi \rangle / 2$ can be calculated. The final result is

$$\langle S_x \rangle = \qquad (15)$$

$$\frac{1}{2\xi}\left[c_x \cos 2\vartheta + \left(\frac{\xi c_y}{c_z}\sin\phi + \frac{\gamma\chi_z c_x}{c_z}\cos\phi\right)\sin 2\vartheta\right],$$

$$\langle S_y \rangle = \qquad (16)$$

$$\frac{1}{2\xi}\left[c_y \cos 2\vartheta - \left(\frac{\xi c_x}{c_z}\sin\phi - \frac{\gamma\chi_z c_y}{c_z}\cos\phi\right)\sin 2\vartheta\right],$$

$$\langle S_z \rangle = \frac{1}{2\xi}\left(\gamma\chi_z \cos 2\vartheta - c_z \cos\phi \sin 2\vartheta\right). \qquad (17)$$

Here $c_x = (\gamma\chi_x + \alpha k_{||}\sin\varphi)$, $c_y = (\gamma\chi_y - \alpha k_{||}\cos\varphi)$, and $c_z = \sqrt{\xi^2 - \gamma^2\chi_z^2}$. Using the components (15)–(17) one can draw the spin surface in the spin space by varying the parameters in the range $\vartheta = (0 - \pi/2)$ and $\phi = (0 - 2\pi)$. Figure 2 shows an example of the spin surface. The geodesic lines that run over the surface and the location of the poles on the surface depend on the parametrization scheme used and are helpful in visualizing the surface itself. Different parametrization schemes will give different families of the geodesic lines, however, the topology of the surface will not change. It can be shown that the lines in Fig. 2 rotate in concert with $\mathbf{k}$. The important property of the surface shown in Fig. 2 is that it possesses exactly the spherical symmetry, independent of direction of $\mathbf{k}$ and semiconductor parameters. It appears that the radius of the sphere is equal to $1/2$. This can be proved by calculating the square of the radius. After rather lengthy algebraic manipulations (for this purpose the computer algebra package *Mathematica* has been used) one can prove that

$$|\langle \mathbf{S} \rangle|^2 = \langle S_x \rangle^2 + \langle S_y \rangle^2 + \langle S_z \rangle^2 = \frac{1}{4}. \qquad (18)$$

This means that for separate as well as for combined Rashba and Dresselhaus Hamiltonians the spin surface in the spin space in all cases is the sphere of radius $1/2$. This has not been evident at the first glance, since the spin splitting of the bands is related to spin–orbit interaction and, as a result, with the noncommutativity of the spin and Hamiltonian operator (5). In such cases one would expect that the helicity rather than spin quantum numbers are more appropriate in the problem. Earlier we have shown [4–7] that in valence bands of cubic semiconductors, where spin–orbit interaction is strong and as a result the rearrangements of the band

spectrum takes place at the Brillouin zone centre, the hole spin surfaces are the spheroids.

The property that the spin surface has the spherical shape for all electron wave vectors may be advantageous in practical calculations. Since the spin surface is spherical, the parameterization of the spinor can be performed in the initial σ_z representation that has been used to construct the initial Hamiltonian rather than calculating the unitary matrix, switching over to the energy representation, and then back to σ_s representation. In this case the knowledge of the unitary transformation matrix is not required and the spin quantization axis or spin direction can be selected directly in the σ_z representation.

In conclusion, despite of the nonsphericity of free electron conduction band in A_3B_5 and A_2B_6 semiconductors, it is shown that the spin surface has exactly the spherical shape for separate Rashba and Dresselhaus Hamiltonians, as well as for a combined Rashba–Dresselhaus Hamiltonian. Therefore, in contrast to valence band holes, one has that for a free electron all directions of the spin quantization axis in cubic semiconductors are equivalent.

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LAISVOJO ELEKTRONO SUKINYS KUBINIUOSE PUSLAIDININKIUOSE

A. Dargys

Puslaidininkių fizikos institutas, Vilnius, Lietuva

Santrauka

Kvantiniai sukinio paviršiai nusako pagrindines laisvojo elektrono bei skylės sukinio savybes, įskaitant superpozicines būsenas, kai yra fiksuotas elektrono (skylės) bangos vektorius ir apibrėžta energijų juosta. Kadangi sukinio ir orbitos sąveika puslaidininkiuose yra baigtinė, manoma, kad sukinių paviršiai turėtų būti sferoidai (sukimosi elipsoidai). Valentinės juostos atveju šis teiginys buvo įrodytas darbuose [4–7]. Šiame straipsnyje parodyta, kad kubiniuose puslaidininkiuose, pavyzdžiui A_3B_5 ir A_2B_6 junginiuose, nepaisant baigtinės sukinio ir orbitos sąveikos, visais atvejais laidumo juostos elektronų sukinių paviršiai yra ne sferoidai, o sferos, t. y. sukinio paviršiai nepriklauso nuo elektroninės bangos sklidimo krypties bei parametrų, nusakančių laidumo juostos savybes. Ši universali elektrono sukinio savybė kubiniuose puslaidininkiuose gali palengvinti tiek energinių juostų, tiek su sukiniu susietų savybių skaičiavimus dvimačiuose dariniuose tuo atveju, kai reikia atsižvelgti į erdvinį kvantavimą.