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Spin eigen-states of Dirac equation for quasi-two-dimensional electrons

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ABSTRACT

Dirac equation for electrons in a potential created by quantum well is solved and the three sets of the eigen-functions are obtained. In each set the wavefunction is at the same time the eigen-function of one of the three spin operators, which do not commute with each other, but do commute with the Dirac Hamiltonian. This means that the eigen-functions of Dirac equation describe three independent spin eigen-states. The energy spectrum of electrons confined by the rectangular quantum well is calculated for each of these spin states at the values of energies relevant for solid state physics. It is shown that the standard Rashba spin splitting takes place in one of such states only. In another one, 2D electron subbands remain spin degenerate, and for the third one the spin splitting is anisotropic for different directions of 2D wave vector.

1. Introduction

Exploiting the spin degree of freedom of charge carriers (electrons or holes) seemed impossible up to relatively recent times. At present it is the main aim of the new branch of electronics, called "spintronics" [1]. Controlling particle spin is possible because of the spin–orbit interaction, which binds the spin and momentum of a particle in an external inhomogeneous potential. Theoretical and experimental study of this problem is very important, in particular, for the study of layered semiconducting heterostructures, or quantum wells, in which charge carriers confined by the

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potential of some narrow layer, represent practically two-dimensional (2D) electron gas. In the presence of the anisotropy determined by the applied electric field and/or special configuration of the heterostructure, when the anisotropy is transversal to this layer, spin–orbit interaction removes spin degeneracy of the 2D conducting or valent band [1,2]. This phenomenon is known as Rashba effect [3,4].

A plane potential well is one of the mostly used models to study the properties of quasi-2D electron gas. Non-relativistic problem is solved for the electron propagation in the external potential which is inhomogeneous in one direction and homogeneous in two other directions, taking into account the potential relief. If the potential has the form of the well (in the simplest case of the rectangular potential box) in the direction of inhomogeneity, electrons are confined by this potential layer. They preserve the momentum in the plane of the layer and fill in discrete energy levels of the spacial quantization, whose number is determined by the depth of the potential well. In the result, such layer (interface) is characterized by the set of the 2D electron bands. In the non-relativistic approximation the dispersion laws of these bands are determined by the solutions of the Schrödinger equation which contains spin–orbit interaction. As it was mentioned above, spin–orbit interaction determines spin orientation. In the case of an asymmetric quantum well, it determines Rashba dispersion law, or band splitting in the **k**-space depending on spin direction.

It is well known that the existence of the electron spin is a natural consequence of the relativistic Dirac equation (DE) [5], and that spin–orbit interaction in Schrödinger equation results from the expansion of Dirac equation with respect to the degrees of $1/c$ [6–8]. A particle wavefunction $\Psi(\mathbf{r})$ in Dirac quantum theory is a four-component coordinate function which is represented in the form of a matrix which contains one-column (bispinor) coordinate functions. In this theory the operators related to the spin of a particle, are sixteen 4×4 Dirac matrices, including the unit matrix. In the non-relativistic approximation bispinor wavefunction is approximated by a spinor one. In this case the operators of the spin projections are given by the three Pauli matrices. Usually it is assumed that Schrödinger equation which includes spin–orbit interaction, takes into account all possibilities of Dirac equation. Nevertheless, the question, how completely and exactly non-relativistic approximation describes the spin degree of freedom, remains open. This problem is of special importance at present when the perspectives of exploring particle spin in the processes of information storage and transfer, become realistic.

In the present paper we solve Dirac equation with asymmetric rectangular potential which models a quantum well. Dirac equation with rectangular (step-like or box-like) potential was studied in various papers starting with the famous paper of Klein [9]. Mostly, these papers deal with 1D electron propagation, perpendicular to the rectangular step, with the main attention devoted to the role of the relativistic effects [9–12] or to the role of specific potentials which capture particles. In particular, in [13] this potential was represented in the form of a spatial dependence of a mass of a relativistic particle, and in [14] a quaternion potential was studied.

Below we study the spin states of quasi-2D of electrons in a quantum well, and calculate their energies as functions of their 2D wave vectors. The corresponding solutions are analyzed for the values of energies relevant to important problems of solid state physics, and compared with the results of non-relativistic model. For convenience and completeness of the paper we give some known results from the theory of Dirac equation.

2. Dirac equation

Stationary Dirac equation for a particle in the absence of the magnetic field has the form [5–7]

$$\left[c\hat{\boldsymbol{\alpha}}\mathbf{p} + V(\mathbf{r}) + \hat{\beta}mc^2\right]\Psi = E\Psi. \tag{1}$$

Here c is the speed of the light, m is the mass of a particle, $\mathbf{p} = -i\hbar\nabla$ is its momentum operator, $\hat{\boldsymbol{\alpha}} = \sum_j \mathbf{e}_j\hat{\alpha}_j$, $\hat{\alpha}_j$ $(j = x, y, z)$ and $\hat{\beta}$ are Dirac matrices, $V(\mathbf{r})$ is the external potential, and $\Psi(\mathbf{r})$ is a four-component coordinate function introduced above. Dirac matrices satisfy the following