Annals of Physics 369 (2016) 85–101

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

General solution of the Dirac equation for quasi-two-dimensional electrons

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ARTICLE INFO

Article history:
Received 1 December 2015
Accepted 21 March 2016
Available online 26 March 2016

Keywords:
General solution of the Dirac equation
Spin state
Rashba spin splitting
Spin–orbit interaction
Quantum well
Two-dimensional electron gas

ABSTRACT

The general solution of the Dirac equation for quasi-two-dimensional electrons confined in an asymmetric quantum well, is found. The energy spectrum of such a system is exactly calculated using special unitary operator and is shown to depend on the electron spin polarization. This solution contains free parameters, whose variation continuously transforms one known particular solution into another. As an example, two different cases are considered in detail: electron in a deep and in a strongly asymmetric shallow quantum well. The effective mass renormalized by relativistic corrections and Bychkov–Rashba coefficients are analytically obtained for both cases. It is demonstrated that the general solution transforms to the particular solutions, found previously (Eremko et al., 2015) with the use of spin invariants. The general solution allows to establish conditions at which a specific (accompanied or non-accompanied by Rashba splitting) spin state can be realized. These results can prompt the ways to control the spin degree of freedom via the synthesis of spintronic heterostructures with the required properties.

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http://dx.doi.org/10.1016/j.aop.2016.03.008
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1. Introduction

Study of the spin degree of freedom is an important problem not only for fundamental physics, but for practical applications also, in view of the last advances of nanotechnologies and promising perspectives of the new branch of electronics called spintronics [1]. Of the special interest is spin behaviour in quasi-two-dimensional structures [2], such as layered semiconducting heterostructures, quantum wells (QW) and noble-metal-based surface alloys [3]. The gigantic spin splitting has been reported to take place in bismuth tellurohalides, widely used in modern micro- and nanoelectronics [4–6]. In these systems there exist such phenomena as band spin splitting, or Rashba effect [7,8], spin Hall effect etc. These phenomena are caused by spin–orbit interaction (SOI), which is manifested when particles propagate in an inhomogeneous potential. Therefore, the detailed study of the spin degree of freedom, the very existence of which is the direct consequence of the Dirac equation (DE), is important.

Many problems of solid state electronics are usually studied within the Schrödinger equation (SE) taking into account SOI which appears in the Hamiltonian as the relativistic Thomas correction after the transition in DE to the non-relativistic limit [9–11]. This correction takes the simplest form of the SOI operator in the case of a spherically symmetric field, and the form of Rashba SOI for two-dimensional (2D) carriers in the field of a plane well.

It is generally assumed that SE with SOI operator describes all possible cases of entangling of coordinate and spin variables. Worth noting that DE does not include a separate term responsible for SOI. Its appearance in the nonrelativistic approximation reflects the fact of the hidden coupling between the particle's degrees of freedom in the DE. The corresponding relation results from the fact that spatial and spin coordinates are not separated in the DE. This is very clear if one searches the solution of the DE for a free particle in the system of eigen functions that is consistent not with the momentum operator, but with the operator of the total angular momentum.

To study how complete is the description of the spin degree of freedom within the nonrelativistic approximation, the solution of the DE for electrons in the field of the plane QW was recently analysed in [12] with the subsequent consideration of nonrelativistic energies. It has been found, somehow unexpected, that there are *four* independent solutions which correspond to also four different eigen spin states with different spin polarizations – in other words, with different axes of spin momentum quantization – and with different characters of SOI manifestation. Nonetheless, from the mathematical point of view there is nothing strange in this, according to the theory of linear differential equations.

Indeed, the DE is, in fact, the system of four equations for the components $\psi_1, \ldots, \psi_4$ of the Dirac bispinor. In the external potential which varies in one direction only (for instance, along z-axis), when the space in the two other directions is homogeneous, particle states can be characterized by certain value of the 2D momentum $\mathbf{k}_\perp = \mathbf{e}_x k_x + \mathbf{e}_y k_y$. Then the dependence of the wavefunction on the spatial coordinates x and y is determined by the standard exponential term $\exp i\left(k_x x + k_y y\right)$, and DE transforms into the system of four ordinary differential equations for functions $\psi_j(z)$ $(j = 1, \ldots, 4)$ of one variable. In this case one can find exactly four linear mutually independent sets of functions $\psi_{\nu,1}, \ldots, \psi_{\nu,4}$ $(\nu = 1, \ldots, 4)$, which represent the solution of the latter system of equations [13]. Such linearly independent solutions form *the fundamental system* of solutions. For the system of solutions found in [12], the Wronskian does not vanish, $\mathrm{Det}|\psi_{\nu,j}(z)| \neq 0$, what unambiguously proves that the solutions are linearly independent and represent the fundamental system of solutions of the DE. Any linear combination of them with arbitrary coefficients is also the solution of the DE [13]. Such a solution of the system of equations is called *general*, and, naturally, should contain some free parameters, whose variation continuously transforms one solution into another.

Though different solutions correspond to different spin states, any variation of the free parameters means an arbitrary rotation of the spin polarization, which in turn leads to the appearance of SOI, different for each state. This is why it is important to find the general solution, or in other words, the solution with free parameters, when considering the DE for the specific physical situation. This solution, being a unique one, independently on the existence of the spin invariants, would allow to determine conditions at which a specific spin state is realized, and, hopefully, would open new possibilities of the control of the spin degree of freedom. Below we consider quasi-2D electrons kept by an asymmetric QW, and find the general solution of the DE. The effect of their spin polarization on the energy spectrum is also analysed.

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