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Spin-splitting of electron subbands in semiconducting films with a variable band gap

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Abstract

We investigate size-quantized electron states in a film (quantum well) with a variable band gap, based on compounds of $Pb_{1-x}Sn_xSe$ type. It is shown that an asymmetric modulation of the gap width in the direction of the growth of the film generally leads to spin-splitting of electron subbands. We discuss the influence of surface properties on the magnitude of the electron's spontaneous polarization. Finally, we point out some peculiar degeneracies of the spectrum, caused by particular boundary conditions.
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1. Introduction

The possibility of the electron spin utilization in nanosize semiconductor devices has been a subject of active investigations for a long time [1]. Recently this problem became especially attractive in connection with the growing technological potential to synthesize structures with given parameters. One of the central problems of spintronics is the experimental realization of the source of polarized electrons (spin filter). Until recently, only ferromagnetic metals [2] and magnetic semiconductors [3] have been used as the basis materials for a device application. From the technological point of view, however, it is more preferable to use nonmagnetic materials. The spin filter, based on a wide gap semiconductor, three barrier structure was proposed by Koga et al. [4]. The filter made from GaInAs asymmetric quantum well was discussed in Ref. [5] (see also Ref. [6]). The main principle of these devices is a utilization of Rashba's effect for spin-splitting of the resonant levels, that in principle allows the blocking of one of the tunneling channels (with a given spin projection). In reality, however, the efficiency of such sources turns out to be low, since Rashba's effect, being perturbative in its nature, cannot lead to a large separation of spin-split levels.

The implication of narrow-gap semiconductors with strong spin–orbit interaction as basis materials may significantly improve the characteristics of existing sources of polarized electrons, based on nonmagnetic materials. In the previous study [7], for instance, the large spin-splitting of the spectrum of asymmetric HgTe quantum wells was reported. Theoretical investigation of similar effects in an asymmetric quantum heterostructure containing lead salt compounds was performed by Hasegawa et al. [8].

However, up to now all authors focused on studying layered systems, such as quantum wells, grown on different substrates. It is, therefore, of interest to investigate electronic properties of inhomogeneous structures, e.g. solid alloys. In the present work,

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we study the size-quantized spectrum of a film with variable energy gap, which may be easily formed from compounds of the $Pb_{1-x}Sn_x(S, Se)$ type grown in the $\langle 111 \rangle$ direction. It is known [9,10] that the variation of the fraction x in the mentioned alloys mainly leads to the variation of the forbidden band width. Therefore, it is possible to create structures via spatial modulation of the fraction. For instance, the bulk $Pb_{1-x}Sr_xSe$ compounds were experimentally realized and investigated by Wu et al. [11]. We will focus on the one-dimensional energy gap modulation in $\langle 111 \rangle$ direction. Then, the problem of an electron moving in the infinite crystal possesses a hidden symmetry and may be reformulated in supersymmetrical form [12]. The presence of crystal boundaries leads generally to destruction of the supersymmetry. However, there exists a class of boundary conditions for which it survives, but is spontaneously broken.[1] In what follows, we consider the simplest, but still illustrative case for which the forbidden band width varies linearly in the direction of the growth of the film. In this case, the electron and hole dispersions can be found exactly. We will also assume that confinement in the film has a general character because of the large work function.

2. Effective Hamiltonian for the electron in bulk lead salt compounds and boundary conditions

The electronic spectrum (near the L—point of the Brillouin zone) of lead salts and solid alloys based on them is most accurately described in terms of Dimmock's model [10,13]. Neglecting the anisotropy of the parameters, we can write the Hamiltonian of the model as:

$$H = \left(\frac{p^2}{2m} + \frac{\varepsilon_g}{2}\right)\beta + s(\vec{\alpha} \cdot \vec{p}). \tag{1}$$

Here, $\vec{\alpha} = (\alpha_x, \alpha_y, \alpha_x)$ and β are Dirac's matrices, ε_g is energy gap width, and $s = P/m_0$ is a characteristic velocity which is proportional to the matrix element P of the momentum between the extremal valence and conduction band states (m_0—free electron mass). The envelope ψ of the wavefunction is a 4-spinor by its transformational properties. The first term in Eq. (1) describes the contribution of remote bands in the second order of perturbation theory; m is the corresponding effective mass. It is necessary to note that in the Hamiltonian model in Eq. (1), the spin–orbit interaction is taken into account exactly.

The form of the Hamiltonian in Eq. (1) implies the existence of three intervals on the energy scale: (i) "Nonrelativistic" regime: the momentum $p \ll \varepsilon_g/s$; (ii) Intermediate energies, when $p \sim \varepsilon_g/s$, but the first term in Eq. (1) is small, compared to the others; (iii) High energies, when the quadratic term in Eq. (1) dominates. The existence of the interval (ii) can be proved by the following argumentation. Let a be the size of the domain, where the particle is confined. Then the requirement that $p^2/2m \ll \varepsilon_g, ps$ leads to the following constraint for the size of the system: $a \gg 1$ nm, which is obviously the condition of applicability of the effective mass approximation. In what follows, we will assume that the excitation energy is in the range (ii).

In the bulk material, the electron wavefunction is a plane wave and the electron dispersion is given by $\varepsilon = ((sp)^2 + (p^2/2m + \varepsilon_g/2)^2)^{1/2}$. For a given energy, $\varepsilon > \varepsilon_g/2$, there always exist four waves: two propagating and two evanescent. Under the condition $m > \varepsilon_g/s^2$ (which is satisfied by lead salts) the localization length of evanescent waves ($\sim \hbar/ms$) is smaller than the wavelength of propagating modes [14]. Thus, in the bulk of the system we can neglect the overlapping of modes which are strongly localized near the surface. For energies in range (ii), the wavefunction in the bulk will be determined by the Hamiltonian from Eq. (1) with the quadratic term being ignored. Near the surface it is necessary to retain the higher derivative term in Eq. (1). Localized modes will now determine the effective boundary condition (BC) at the surface of the system for propagating waves.

The most general form of the BC, which is allowed by the Hamiltonian in Eq. (1) and makes the current vanish at the surface Σ of the system, is

$$(\hbar/ms)\partial\psi/\partial n + \mathbf{\Lambda}(E_g, \varepsilon_g, m)\psi = 0, \tag{2}$$

where $\mathbf{\Lambda}$ is some (in general, nonsingular) matrix, which is determined, in particular, by the energy gap width outside (E_g) and inside (ε_g) the system. We will assume that electrons remain localized inside the allowed domain at all energies, which corresponds to the inequality $E_g \gg \varepsilon_g$. Under this condition, $\mathbf{\Lambda} \sim [E_g/ms^2]^{1/2}$ and the BC from Eq. (2) goes over into $\psi|_\Sigma = 0$ [14]. If, in addition, $\varepsilon_g \ll ms^2$, then it is easy to write down an effective BC only for propagating waves in the form:

$$\mathbf{B}\psi|_\Sigma = 0, \tag{3}$$

where $\mathbf{B}$ is some singular matrix[2] (see also [15,16]). It is important to note that the BC, Eq. (3), acts not at the very surface of the system, but at the boundary of the thin layer, $\sim \hbar/ms$ thick, located at the surface. In the bulk the wavefunction is described by the two-band Dirac's Hamiltonian:

$$H = s(\vec{\alpha} \cdot \vec{p}) + (\varepsilon_g/2)\beta. \tag{4}$$

[1] This general issue will be discussed separately elsewhere.

[2] It must be emphasized that BC in Eqs. (2) and (3) account for band mismatch inside and outside the system. The mentioned asymptotic of $\mathbf{\Lambda}$ is valid only in the absence of the band mismatch.

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