The spin polarization of conduction electrons in boundary states

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The value of the spin polarization $\langle S \rangle_0$ of the two-dimensional boundary electron current in HgTe is estimated. The quantity $\langle S \rangle_0$ does not contain the small spin-orbit coupling parameter, since the nondegenerate spectrum of boundary states is formed by the spin-orbit interaction itself.

The spin-orbit coupling of two-dimensional electrons in a heteroboundary field packing an inversion center is generally included in the single-zone effective Hamiltonian as[1]

$$\hat{H} = \frac{\vec{K}^2}{2m^*} + \alpha\hat{\vec{\sigma}}[\vec{K} \times \vec{n}]. \tag{1}$$

Here $\vec{n}$ is the vector normal to the heteroboundary, $\hat{\vec{\sigma}}$ are the Pauli matrices, and $\vec{K}$ is the two-dimensional momentum of a charge carrier. Under typical subzone filling conditions the ratio of the spin splitting of the spectrum at the Fermi level to the value of the Fermi energy $\delta = \alpha K_F / E_F$ is a small parameter. In the case of a nondegenerate spectrum the Kramers correlation of the spin state of an electron with the direction of its two-dimensional momentum $E\uparrow(\vec{K}) = E\downarrow(-\vec{K})$ leads to the possibility of spin polarization of the electron subsystem by a longitudinal electric current.[2] The value of the induced spin, found in Ref. 2 using the model (1), divided by the number of nonequilibrium electrons, gives the polarization $\langle S \rangle = \delta$. Therefore, the spin polarization is as small as δ.

However, it is known that for semiconductors which contain atoms of heavy elements there is an alternative possibility of realizing a nondegenerate two-dimensional electron subsystem.[3,4] Solutions of this type—boundary states (BS)—arise in the matching at the heteroboundary of the wave functions corresponding to matrix Hamiltonians with differing zone parameters and, as a rule, represent a combination of states of different zones, shifted by the strong perturbing potential of the heteroboundary. When the contribution of the spin-orbit interaction to the formation of the quasiparticle zone parameters is large, for example, for a large spin-orbit splitting of the valence band, nondegenerate branches can appear in the energy spectrum of the heteroboundary. The origin of these branches cannot be attributed to the weak spin splitting of the existing bulk branches of the spectrum of the type (1). In fact, nondegenerate BS are formed by the strong spin-orbit coupling itself at the heteroboundary, where often for a given momentum $\vec{K}$ the spectrum contains only a single component of the spin doublet.[4] The value of the spin polarization of electrons in such states must clearly be determined by the BS zone parameters and should not involve the small parameter δ. In the simplest case of a parabolic BS spectrum the spin polarization will be determined by the mean value of the spin in an isolated boundary state $\langle S \rangle_0$.

A parabolic BS spectrum can apparently be realized in the heterotransitions CdTe–HgTe or CdTe–αSn. The Fermi level of such a system, related to the top of the valence band of a gapless semiconductor (the representation Γ_8), penetrates deeply inside the band gap of CdTe ($\Delta_v \sim 350$ meV), so in a small energy range near E_F the BS wave function can be assumed to be concentrated entirely in the gapless semiconductor which occupies the region $x > 0$. The 4×4 Luttinger matrix Hamiltonian,[5] which describes the charge carrier spectrum in the representation Γ_8, must be augmented, in the absence of penetration of the wave function inside the barrier, by zero boundary conditions on each of the four components of the envelope wave function Ψ. The spin polarization can be determined by choosing a coordinate system with axes $x \| \vec{n}$ and $y \| \vec{K}$, in which the spin states with opposite z-polarization, according to (1), will be split. Since $\hat{k}_z \Psi = 0$, the Luttinger Hamiltonian $\hat{H}_L$ can be reduced to subdiagonal form:

$$\hat{H}_L = (\gamma_1 + \frac{5}{2}\gamma)\hat{\vec{k}}^2 - 2\gamma(\hat{\vec{K}}\hat{\vec{J}})^2$$

$$= \begin{bmatrix} \hat{H}_1 & 0 \\ 0 & \hat{H}_{-1} \end{bmatrix}; \quad \hat{H}_\mu = \begin{bmatrix} (\gamma_1 + \gamma)\hat{\vec{k}}^2 & \sqrt{3}\gamma\hat{k}_{-\mu}^2 \\ \sqrt{3}\gamma\hat{k}_\mu^2 & (\gamma_1 - \gamma)\hat{\vec{k}}^2 \end{bmatrix}; \quad \begin{array}{l} \hat{\vec{k}} = -i\vec{\nabla} \\ \hat{k}_\mu = \hat{k}_x + i\mu\hat{k}_y. \end{array} \tag{2}$$

The four degenerate eigenfunctions of the operator $\hat{\vec{J}}$ for angular momentum 3/2, which are used as the basis of the representation Γ_8, were chosen in the form

$$\begin{array}{ll} \{|\frac{3}{2}> = \frac{1}{\sqrt{2}}(X + iY)\uparrow; & |-\frac{1}{2}> = \frac{1}{\sqrt{6}}[(X - iY)\uparrow + 2Z\downarrow]\}_{\mu=1} \\ \{|-\frac{3}{2}> = \frac{1}{\sqrt{2}}(X - iY)\downarrow; & |\frac{1}{2}> = \frac{1}{\sqrt{6}}[(X + iY)\downarrow - 2Z\uparrow]\}_{\mu=-1} \end{array}, \tag{3}$$

which corresponds to the representation of the matrices $\hat{J}_\alpha$ in the form of the following direct product:

$$\hat{J}_\alpha = \hat{\sigma}_\alpha \times \hat{j}_\alpha; \quad \hat{j}_x = \begin{bmatrix} 0 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -1 \end{bmatrix}; \quad \hat{j}_y = \begin{bmatrix} 0 & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & 1 \end{bmatrix}; \quad \hat{j}_z = \begin{bmatrix} \frac{3}{2} & 0 \\ 0 & -\frac{1}{2} \end{bmatrix}. \tag{4}$$

The quantum number $\mu = \pm 1$ characterizing the polarization of a state is an eigenvalue of the operator of mirror reflection in the plane of the vectors $\vec{n}$ and $\vec{K}$. The zero boundary conditions $\Psi(x=0) = 0$ do not mix spin states of different parity μ. This, however, concerns any boundary condition of the envelope method which use only the parameters of the bulk Hamiltonians and which does not involve the microstructure of the boundary. However, if the (xy) plane also serves as the symmetry plane of the crystal, the assumption that the boundary conditions conserve the parity μ is completely justified. Here the solution of the problem (2) simplifies considerably and gives a parabolic branch of nondegenerate BS of the electron type,[6,7] shown in Fig. 1. The doubly degenerate bulk branches of the spectrum of electrons $E_e = (\gamma_1 + 2\gamma)K^2 = K^2/2m_e$ and heavy holes $E_h = (\gamma_1 - 2\gamma)K^2 = -K^2/2m_h$ are shown in Fig. 1 by the dashed line (in a gapless semiconductor $2\gamma > \gamma_1$). For $K \uparrow\uparrow y$ a BS exists only for the single sign $\mu = +1$. For the chosen location of the heterostructure layer the second submatrix of the Hamiltonian $\hat{H}_{(-1)}$ gives solutions in the form of BS for $\vec{K} \uparrow\downarrow y$. The wave functions Ψ_μ of the BS found transform into each other under time reversal and form a Kramers doublet:

$$\Psi_\mu = \frac{1}{\sqrt{1+B^2}} \begin{pmatrix} 1 \\ B \end{pmatrix}_\mu (e^{-q_e x} - e^{-q_h x}) e^{iKy}, \tag{5}$$

where $B = (\sqrt{3} + \sqrt{\beta}/\sqrt{3\beta} - 1)$; $q_e = (\mu K/2)(1 + \sqrt{3\beta})$; $q_h = (\mu K/2) \times (\sqrt{(3/\beta)} - 1)$, and $\beta = m_e/m_h$ is the ratio of the electron and heavy hole masses in a gapless semiconductor. Since the Hamiltonian (2) commutes with the operator $[\hat{\vec{r}} \times \hat{\vec{k}}] + \hat{\vec{J}}$, the matrix operator $\hat{\vec{J}}$ plays the role of the quasiparticle spin, and its expectation value in the boundary state (5) will determine the polarization:

$$< J_x >=< J_y >= 0;$$

$$< J_z >= \frac{\mu}{1+B^2}\left(\frac{3}{2} - \frac{1}{2}B^2\right) = -\mathrm{sign}(K_y)\sqrt{\beta}\frac{\sqrt{3}-\sqrt{\beta}}{1+\sqrt{\beta}}. \tag{6}$$

In the rotation of the vector $\vec{K}$ by the angle θ in the plane of the heteroboundary $\langle J_z \rangle_\theta = \langle J_z \rangle_{\theta=0} \cos\theta$, $\langle J_y \rangle_\theta = \langle J_z \rangle_{\theta=0} \sin\theta$. We note that the states Ψ_μ transform into each other under rotations $\theta = \pm\pi$. The extremal value is $\langle J_z \rangle = 0.5$ for $\beta = 1/3$. In HgTe $\beta = 0.063$ and $\langle J_z \rangle = 0.35$.

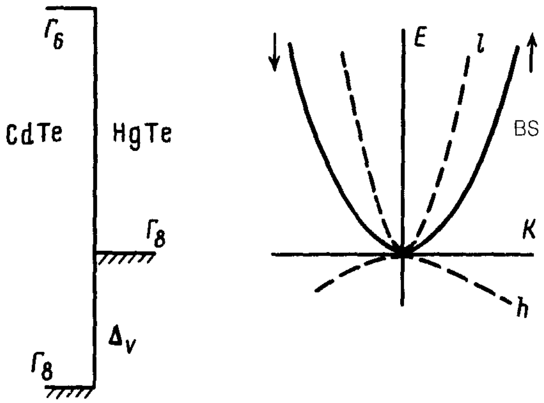

FIG. 1.

However, the quantity $\langle J_z \rangle$ does not characterize the spin polarization itself, since it also includes, according to (3), the mean value of the microscopic orbital angular momentum of the hole. We can find the spin polarization $\langle \sigma_z/2 \rangle$ by averaging over the orbital parts of the basis functions in (3). We obtain

$$< \frac{\sigma_x}{2} >=< \frac{\sigma_y}{2} >= 0; \ < \frac{\sigma_z}{2} >=< \frac{J_z}{3} >. \quad (7)$$

Which of the quantities $\langle J_z \rangle$ or $\langle \sigma_z/2 \rangle$ plays the role of $\langle S \rangle_0$ depends on the actual experimental setup. For example, in a structure like the planar field transistor, which contains ferromagnetic source and sink contacts magnetized in the z direction and which plays the role of a polarizer and analyzer,[8] the nonreversibility in the current transfer apparently is determined by the spin polarization $\langle \sigma_z/2 \rangle$, while in experiments with polarized light the main parameter is the mean total angular momentum $\langle J_z \rangle$. The possibility of efficient injection from ferromagnetic electrodes has recently been confirmed experimentally.[9]

It should be noted that control of the spin polarization in heterostructures is possible not only by means of a longitudinal current. The restoration of the inversion symmetry in a double heterostructure (a quantum well) implies, in particular, that BS with opposite spin polarization and the same two-dimensional momentum are realized on the second heteroboundary of the structure. The wave functions of the components of such a spin doublet are related by the product of the inversion and time reversal operators, and the maxima of the spin density are spatially separated. Clearly, under these conditions the transverse electric field induced, for example, by a closed Schottky barrier will lead to lifting of the restored degeneracy and to spin polarization of the electron flux from the source to the sink. Because of the quantum dimensional effect, a double heterostructure also permits the effect of unpolarized bulk states of the l-band to be tuned out.

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