Surface states in a gapless semiconductor

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It is shown that gapless α-Sn and HgTe semiconductors have specific surface states, which are a superposition of the electron states in the valence band and in the conduction band. The effective mass, which determines the motion along the surface in these states, depends on the mass ratio of the free electron and the free hole.

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Additional branches of the electronic spectrum, which are attributable to the surface states, exist, as we shall show, in a gapless semiconductor with an inverse band structure.[1] The wave function of an electron in such a state vanishes at the surface, has a maximum at a certain distance from it and falls off exponentially deep into the crystal. The characteristic scale of variation of the wave function in the perpendicular direction to the surface is of the order of $1/k$, where k is the wave vector along the surface. The surface states under consideration, therefore, can be described within the context of the effective-mass method. As far as we know, this is the only case in which such analysis of the surface states is possible.

The electronic spectrum of a gapless semiconductor near the degeneracy point of the bands is described by the Luttinger Hamiltonian[2]

$$H = \frac{1}{2m_0}\left[\left(\gamma_1 + \frac{5}{2}\gamma\right)\mathbf{p}^2 - 2\gamma(\mathbf{pJ})^2\right], \tag{1}$$

where $\mathbf{p}$ is the quasi-momentum operator and J_x, J_y and J_z are the 4×4 matrices that correspond to the 3/2 moment. We shall limit ourselves to the spherical approximation. The effective masses of the electron and the hole are given by the expressions $m_e = m_0/(\gamma_1 + 2\gamma), m_h = m_0/(2\gamma - \gamma_1)$. Here m_0 is the mass of a free electron, $\gamma = (2\gamma_2 + 3\gamma_3)/5$, and $\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters. It is assumed that $y_1 + 2y = 0$ and $2y - y_1 > 0$.

Suppose that the crystal occupies a region $z > 0$. The surface states are described by the solutions of the equation $H\psi = E\psi$, which satisfy the boundary condition $\psi(0) = 0$ and which decrease as $z \to \infty$. Suppose that the wave vector k in the surface plane is directed along the x axis. For the specified values of k and energy E there are four independent solutions of the Schrödinger equation with the Hamiltonian (1), which decrease as $z \to \infty$: $\phi_\alpha^{(1)}\exp(ikx - \kappa_1 z)$, $\phi_\alpha^{(2)}\exp(ikx - \kappa^2 z)$. The subscript α has two values $\alpha = 1$ and 2 and the positive values κ_1 and κ_2 are expressed in terms of E and k

$$E = \frac{\hbar^2(k^2 - \kappa_1^2)}{2m_e} = -\frac{\hbar^2(k^2 - \kappa_2^2)}{2m_h}. \tag{2}$$

The $\phi_\alpha^{(1)}$ and $\phi_\alpha^{(2)}$ spinors in the representation in which the J_2 matrix is diagonal can be selected in the form

$$\phi_1^{(1)} = \begin{pmatrix} i\lambda_1 \\ 1 \\ -i \\ -\lambda_1 \end{pmatrix}; \qquad \phi_1^{(2)} = \begin{pmatrix} 1 \\ -i\lambda_2 \\ \lambda_2 \\ -i \end{pmatrix}, \tag{3}$$

where $\lambda_1 = k(\sqrt{3})/(2\kappa_1 + k), \lambda_2 = k(\sqrt{3})/(2\kappa_2 + k)$. The $\phi_2^{(1)}$ and $\phi_2^{(2)}$ spinors are obtained from Eq. (3) by substitution $k \to -k$ and by complex conjugation.

The solution, which satisfies the boundary conditions indicated above, apparently has the form

$$\psi = \Phi e^{ikx} (e^{-\kappa_1 z} - E^{-\kappa_2 z}), \tag{4}$$

where the Φ spinor is a linear combination of the $\phi_\alpha^{(1)}$ [or $\phi_\alpha^{(2)}$] spinors with the coefficients $C_\alpha^{(1)}$ and $C_\alpha^{(2)}$, where

$$C_1^{(1)} \phi_1^{(1)} + C_2^{(1)} \phi_2^{(1)} = C_1^{(2)} \phi_1^{(2)} + C_2^{(2)} \phi_2^{(2)}. \tag{5}$$

The system of equations (5) for the C coefficients has a nontrivial solution only for a specific ratio of the values κ_1, κ_2, and k. This ratio together with Eq. (2), determines the $E(k)$ dependence for the surface states. As we can easily see, there are two possibilities: either $C_1^{(1)} = C_2^{(2)} = 0$ and $\lambda_1(\kappa) \times \lambda_2(-\kappa) + 1 = 0$, or $C_1^{(1)} = C_2^{(2)} = 0$ and $\lambda_1(-\kappa)\ \lambda_2(\kappa) + 1 = 0$.

The solution of these equations for the condition (2) depends on the electron-to-hole mass ratio $\beta = m_e/n_h$

$$\kappa_1 = (1 + \sqrt{3\beta})\,|k|/2, \qquad \kappa_2 = (\sqrt{3/\beta} - 1)\,|k|/2 \qquad \text{for } \beta < 3; \tag{6}$$

$$\kappa_1 = (\sqrt{3\beta - 1})\,|k|/2, \qquad \kappa_2 = (\sqrt{3/\beta} + 1)\,|k|/2 \qquad \text{for } \beta > 1/3. \tag{7}$$

Thus, both solutions (6) and (7) are valid in the interval $1/3 < \beta < 3$ and there is only one solution outside of this interval.

The energy spectrum of the surface states is parabolic: $E = \hbar^2 k_2/2m_s$. The effective mass m_s can be determined by substituting expressions (6) and (7) in Eq. (2):

$$\frac{m_e}{m_{s1}} = 1 - \left(\frac{1 + \sqrt{3\beta}}{2}\right)^2 \qquad \text{for } \beta < 3; \tag{8}$$

$$\frac{m_e}{m_{s2}} = 1 - \left(\frac{\sqrt{3\beta} - 1}{2}\right)^2 \qquad \text{for } \beta > 1/3. \tag{9}$$

The branches of the energy spectrum, which correspond to the surface states in a gapless semiconductor, are shown schematically in Fig. 1. The electron-type surface states exist when $\beta < 1/3$; moreover, their effective mass m_{s1} approaches the value

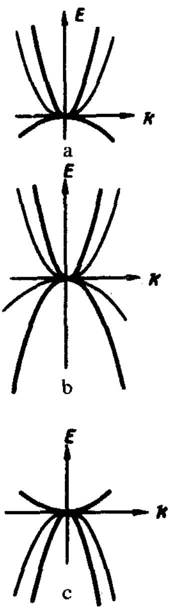

FIG. 1. A spectrum of volume states (heavy lines) and surface states (thin lines) in a gapless semiconductor. (a) $\beta < 1/3$, (b) $1/3 < \beta < 3$, (c) $\beta > 3$.

$(4/3)m_e$ in the limit $\beta \to 0$. At $\beta = 1/3$ the mass m_{s1} becomes infinite and a second branch of the surface states with the mass $m_{s2} = m_e$ splits off from the electronic spectrum of the volume states. There are two types of surface states in the interval $1/3 < \beta < 3$: the electronic states with a mass m_{s2} and the hole states with a mass $m_{s1} < 0$. At $\beta = 3$ the mass m_{s2} becomes infinite and $m_{s1} = -m_h$, so that the hole branch of the surface states merges with the spectrum of the volume states of the holes. Finally, at $\beta > 3$ there is one hole branch of the surface states with the mass $m_{s2} < 0$. The mass m_{s2} approaches the value $-(4/3)m_h$ in the limit $\beta \to \infty$.

The Φ spinors in the expression (4) for the solutions of Eqs. (6), (8), (7), and (9), respectively, have the form

$$\Phi = \begin{pmatrix} ik/|k| \\ \sqrt{\beta} \\ i\sqrt{\beta}k/|k| \\ 1 \end{pmatrix}, \quad \beta < 3; \quad \Phi = \begin{pmatrix} ik/|k| \\ \sqrt{\beta} \\ -i\sqrt{\beta}k/|k| \\ -1 \end{pmatrix}, \quad \beta > 1/3. \qquad (10)$$

The surface states determined by us pertain only to a gapless semiconductor. The Hamiltonian (1) for $y_1 + 2y > 0$, $y_1 - 2y > 0$ describes the spectrum of light and heavy holes in the valence band of an ordinary Ge semiconductor. We can show, however, that the system of Eqs. (5) in this case has only a trivial solution; therefore, the surface states in Eq. (4) do not exist.

The mass ratio is $\beta < 1/3$ in the known, gapless semiconductors. Therefore, only the electron-type surface states can exist in them. Using the value $\beta \approx 0.063$, we obtain $m_s \approx 2m_e$ for HgTe from Eq. (8).

We note that the discrete surface energy levels, which lie below each subband of the Landau electrons, can be expected to appear in the magnetic field that is perpendicular to the surface.

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