Effect of domain structure on the energy spectrum of narrow-gap ferroelectric semiconductors

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(Submitted 30 July 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **56**, No. 5, 268–271 (10 September 1992)

The spectrum of a narrow-gap ferroelectric semiconductor is analyzed. If this semiconductor contains a ferroelectric domain, states localized both at the walls of this domain and inside it split off from the bulk spectrum. These nondegenerate states have a dispersion, in contrast with the "heavy-fermion" states at an isolated domain wall.

Volkov and Pankratov[1] have studied an effect of a domain wall on the spectrum of the ferroelectric phase of a narrow-gap IV–VI semiconductor. They showed that a dispersionless, doubly degenerate state localized at the domain wall arises at the loop of extrema of the bulk bands. They also studied a so-called oppositely directed domain wall: one in which the polarization vector is directed along the normal to the wall. Such walls should have an electric charge. Depending on the sign of this charge, this localized state would arise either at the bottom of the conduction band or at the top of the valence band.

Since a semiconductor is neutral overall, the formation of a domain structure involves the appearance of at least two walls with opposite charges, which bound a domain with a certain polarization. The effect of such a domain on the electronic spectrum of the semiconductor is the subject of the present letter.

In the two-band approximation, the energy spectrum of a ferroelectric semiconductor is described by an equation of the Dirac type:[1,2]

$$\hat{H}\hat{\psi} \equiv [\gamma^0\gamma^3\hat{p}_z + \gamma^0(\vec{\gamma}\cdot\mathbf{k}_\perp) + \gamma^0\Delta(z) + i\gamma^3 u(z) + \varphi(z)]\hat{\psi} = \epsilon\hat{\psi}, \tag{1}$$

where $2\Delta(z)$ and $\varphi(z)$ are the width of the band gap and the work function (both of which depend on the coordinate), the quantity $u(z)$ is proportional to the polarization along the z axis, $\hat{\mathbf{p}} = -i\nabla$, and γ_0 and $\vec{\gamma} = (\gamma^1, \gamma^2, \gamma^3)$ are Dirac matrices. All the energy parameters in Eq. (1) are normalized by division by $\hbar v$, where v is the constant matrix element of the interband transition, and the wave function $\hat{\psi}$ is given by $\hat{\psi} = \tilde{\psi}(z)\exp(i\,\mathbf{k}_\perp\mathbf{r})$, where $(\mathbf{k}_\perp = k_x, k_y, 0)$.

The Hamiltonian $\hat{H}$ commutes with the pseudoparity operator[3]

$$\hat{P} = i\gamma^0\gamma^3(\vec{\gamma}\cdot\mathbf{k}_\perp)/k_\perp, \tag{2}$$

whose eigenvalues are $\lambda = \pm 1$. As the wave functions of (1) we can thus choose eigenfunctions of the operator $\hat{P}$. We thus have $\hat{P}\tilde{\psi}_\lambda = \lambda\tilde{\psi}_\lambda$, and the equation for $\tilde{\psi}_\lambda$ becomes

$$\{\gamma^0[\gamma^3\hat{p}_z + \Delta(z)] + i\gamma^3[u(z) - \lambda k_\perp] + \varphi(z) - \epsilon\}\hat{\psi}_\lambda(z) = 0. \tag{3}$$

Squaring this equation, we find

$$\{\hat{p}_z^2 + \Delta^2(z) + [u(z) - \lambda k_\perp]^2 - [\epsilon - \varphi(z)]^2 + i\frac{d}{dz}[\gamma^3\Delta(z) - \gamma^0\gamma^3\varphi(z) + i\gamma^0 u(z)]\}\hat{\psi}_\lambda(z) = 0. \tag{4}$$

The matrix part of this equation can be diagonalized only if the spatial dependence of the parameters Δ, u, and φ is determined by a common function $f(z)$:

$$\Delta(x) = \bar{\Delta} + \Delta_0 f(z), \quad u(z) = \bar{u} + u_0 f(z), \quad \varphi(z) = \varphi_0 f(z). \tag{5}$$

This diagonalization is carried out with the help of the canonical transformation $\hat{\psi} = \hat{S}\hat{\chi}$, where

$$\hat{S} = \exp(\frac{\alpha}{2}\gamma^0)\exp(i\frac{\beta}{2}\gamma^0\gamma^3),$$

$$\tanh\alpha = \varphi_0/\Delta_0, \qquad \tan\beta = u_0/\sqrt{\Delta_0^2 - \varphi_0^2}. \tag{6}$$

As a result, Eq. (4) acquires the supersymmetric form

$$[\hat{p}_z^2 + W_\lambda^2(z) - i\gamma^3\frac{dW_\lambda}{dz}]\hat{\chi}_\lambda = \tilde{\epsilon}^2\hat{\chi}_\lambda, \tag{7}$$

with a superpotential

$$W_\lambda(z) = \bar{w}_\lambda + \kappa f(z) \tag{8}$$

and a self-energy

$$\tilde{\epsilon}^2 = \epsilon^2 - \bar{\Delta}^2 - (\bar{u} - \lambda k_\perp)^2 + \bar{\omega}_\lambda^2, \tag{9}$$

where $\bar{\omega}_\lambda = [\bar{\Delta}\Delta_0 + (\bar{u} - \lambda k_\perp)u_0 + \epsilon\varphi_0]/\kappa$ and $\kappa = (\Delta_0^2 + u_0^2 - \varphi_0^2)^{1/2}$.

We choose the spatial dependence $f(z)$ to be a square well of width $2a$ with barrier heights $(1 + \mu_L)$ and $(1 + \mu_R)$:

$$f(z) = 1 + \mu_L + \mu_R - (1 + \mu_L)\theta(a + z) - (1 + \mu_R)\theta(a - z). \tag{10}$$

This choice corresponds to a sharp change in the parameters of the semiconductor structure in (5) [$\theta(z)$ is the unit step function]. Solving Eq. (7), we obtain the dispersion relation

$$\tanh(2qa) = \frac{q(q_L + q_R + \kappa_L - \kappa_R)}{(\kappa + \kappa_L)(\kappa + \kappa_R) - q^2 - q_L q_R + q_L(\kappa + \kappa_R) - q_R(\kappa + \kappa_L)}, \tag{11}$$

which is exactly the same as that derived in Ref. 3. Here

$$q_{L,R}^2 = (\bar{w}_\lambda + \kappa_{L,R})^2 - (\bar{w}_\lambda - \kappa)^2 + q^2,$$

$$q^2 = (\bar{w}_\lambda - \kappa)^2 - \tilde{\epsilon}^2 = (\bar{\Delta} - \Delta_0)^2 + (\bar{u} - u_0 - \lambda k_\perp)^2 - (\epsilon + \varphi_0)^2, \tag{12}$$

$$\kappa_{L,R} = \kappa\mu_{L,R}.$$

In the absence of a polarization ($\bar{u}_0 = u_0 = 0$), expressions (8), (9), and (12) reduce to the results for a quantum well formed by semiconductors with mutually inverted bands.[3] In the present letter we are interested in the spectrum of a semiconductor structure which contains electric domains.

An isolated domain wall in a two-band semiconductor leads to the appearance of localized states with an "infinite" mass.[1] The spectrum of these states is doubly degenerate with respect to λ and is bounded in the space of transverse momenta ($k_\perp \leqslant u_0$). The energy is $\epsilon = \pm\bar{\Delta}$, depending on the sign of the charge of the domain wall. These states correspond to a zero mode in supersymmetric Hamiltonian (7).

For simplicity we consider a homogeneous intrinsic semiconductor in which there is a single electric domain in size $2a$. This situation corresponds to $\Delta_0 = \varphi_0 = \bar{u} = 0$, and $\mu_L = \mu_R = 1$ in expressions (5) and (10). Dispersion relation (11) then becomes

$$\tanh(2qa) = \frac{q\sqrt{q^2 - 4\lambda k_\perp u_0}}{2u_0(u_0 + \lambda k_\perp) - q^2}. \tag{13}$$

The roots of this equation determine the energy spectrum of the localized states:

$$\epsilon = \pm\sqrt{\bar{\Delta}^2 + (u_0 + \lambda k_\perp)^2 - q^2}. \tag{14}$$

In the limit $a \to \infty$ (this is the case of two walls separated by an infinite distance), $q = u_0 + \lambda k_\perp$ is a solution of Eq. (13), and the spectrum consists of two degenerate branches with energies $\epsilon = \pm\bar{\Delta}$. If the domain has finite dimensions, the degeneracy with respect to λ is lifted. A straightforward analysis of Eqs. (13) and (14) yields the qualitative spectrum shown in Fig. 1. Solid lines *1* and *2* correspond to states which are localized at the domain walls. We see from this figure that these states exist in the transverse-momentum region $0 \leqslant k_\perp \leqslant u_0$ ($\lambda = +1$) and $0 \leqslant k_\perp \leqslant k_c$ ($\lambda = -1$), where

$$k_c = u_0\left(1 - \frac{\sqrt{1 + 16a^2u_0^2} - 1}{8a^2u_0^2}\right). \tag{15}$$

For negative-parity states at $k_\perp \geqslant k_c$, the solution of dispersion relation (13) becomes purely imaginary, and the wave function converts from an exponentially decaying wave function at the domain walls into an oscillating function. In other words, the dashed line in Fig. 1 corresponds to "quantum-size" states inside the domain. In addition to this branch, a series of "quantum-size" states (the dot-dashed lines in Fig. 1), of negative parity, arise at $k_\perp \geqslant k_{n,c}$, where

$$k_{n,c} = \frac{1}{4u_0}\left(\frac{n\pi}{2a}\right)^2, \qquad n = 1, 2, 3, \ldots. \tag{16}$$

As the dimensions of the domain decrease, and we go to the limit $a \to 0$, we find $k_{n,c} \to \infty$, and these branches disappear. The surface states with $\lambda = +1$ merge into a branch of the bulk spectrum, $\epsilon^- = \pm[\bar{\Delta}^2 = (u_0 - k_\perp)^2]^{1/2}$, while the states with $\lambda = -1$ convert into quantum-size states ($k_c \to 0$) and merge with the branch $\epsilon^+ = \pm[\bar{\Delta}^2 + (u_0 + k_\perp)^2]^{1/2}$. We end up with the ordinary continuous spectrum of a homogeneous ferroelectric semiconductor. In the opposite limit $a \to \infty$, the surface-

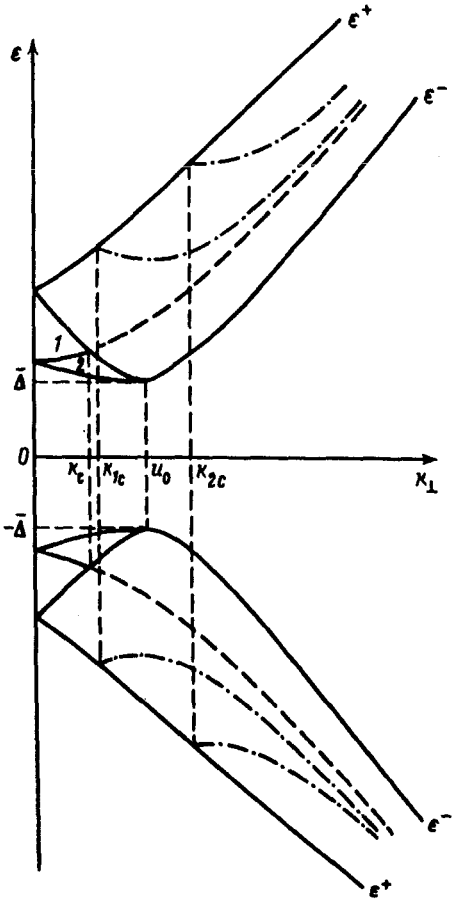

FIG. 1. Electronic spectrum of a ferroelectric semiconductor containing an electric domain. Branches ϵ^+ and ϵ^-—Bulk spectrum of the homogeneous ferroelectric; solid lines *1* and *2*—branches of localized states (localized at domain walls) with positive and negative parities, respectively; dashed and dot-dashed lines—branches of quantum-size states (within the domain) with negative parity.

state branches degenerate into dispersionless branches with an energy $\epsilon = \pm \bar{\Delta}$, while the branches of the quantum-size states converge on the canoncial point ($k_{n,c} \to 0$) and merge with the $\bar{\epsilon}$ branch.

This analysis makes it posible to trace the origin of localized states in a ferroelectric semiconductor upon the formation of a domain structure in this semiconductor. When irregularities associated with variations in the work function and in the width of the band gap are taken into account along with the polarization, the picture is not changed in a qualitative way, as can be seen in the example of an isolated domain wall at an interface between two semiconductors.[4]

We wish to thank B. A. Volkov for useful discussions of these results.

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Translated by D. Parsons