"Heavy fermions" in a supersymmetric ferroelectric domain wall

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The interface between domains in a ferroelectric compound A^4B^6 has two-dimensional electronic states, whose energy is independent of the quasimomentum. These states are nonetheless quantized in a magnetic field. As a result, the surface density of these states oscillates as a function of the field.

The energy spectrum of ferroelectric semiconductors $Pb_{1-x}Sn_xTe$ and $Pb_{1-x}Ge_xTe$ is described by the Dirac Hamiltonian

$$\hat{H} = \begin{pmatrix} \Delta_1 & \vec{\sigma}_\perp \hat{\mathbf{p}}_\perp + \sigma_z(\hat{p}_z + i\Delta_2) \\ \vec{\sigma}_\perp \hat{\mathbf{p}}_\perp + \sigma_z(\hat{p}_z - i\Delta_2) & -\Delta_1 \end{pmatrix}, \tag{1}$$

where σ_z and $\boldsymbol{\sigma}_\perp = (\sigma_x, \sigma_y)$ are the Pauli matrices, $\hat{p}_z = -i\hbar v_\parallel \nabla_z$, $\hat{\mathbf{p}}_\perp = -i\hbar v_\perp(\nabla_x, \nabla_y)$ and Δ_1 is the half-width of the band gap. The perturbation $i\Delta_2$ occurs below the Curie point and is proportional to the sublattice shift **u**. The vector **u** is directed along one of the trigonal axes of the cube, chosen to be the z axis. Hamiltonian (1) is given for the T valley that lies on the same axis. The spinor basis functions $\chi_\mp^{(0)}$ have opposite parities and their phases are shifted by $\pi/2$.

For a homogeneous order parameter $\Delta_2(z) \equiv \Delta$ the spectrum of Hamiltonian (1) is comprised of four branches[1] which are split in spin (Fig. 1);

$$\pm \epsilon_\pm(p_\perp, p_z) = \pm [\Delta_1^2 + p_z^2 + (\Delta \pm p_\perp)^2]^{1/2}, \tag{2}$$

where $p_{z,\perp} \equiv \hbar v_{\parallel,\perp} k_{z,\perp}$, and k_z and $k_\perp = |k_x + ik_y|$ are the longitudinal and transverse quasimomenta. The lifting of band degeneracy due to the loss of the inversion center gives rise to the appearance of an extremum loop[2] but does not change the width of the direct gap.

Because of the large dielectric constant ($\epsilon_0 > 10^3$) and large conductivity, the ferroelectrics A^4B^6 can have oppositely directed domains when the polarization vector ($\propto \mathbf{U}$) is directed at right angles to the plane of the domain wall. In this case, the function $\Delta_2(z)$ changes sign upon crossing the domain wall.[1)]

In the basis $(\chi_-, \chi_+) = (i\sigma_z\chi_-^{(0)}, \chi_+^{(0)})$ Hamiltonian (1) has the form

$$\hat{H} = \begin{pmatrix} \Delta_1 & -i\hat{p}_z + \hat{W}(z) \\ i\hat{p}_z + \hat{W}(z) & -\Delta_1 \end{pmatrix}, \tag{3}$$

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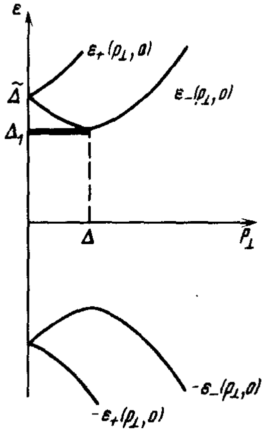

FIG. 1. Energy spectrum of a crystal with a supersymmetric domain wall. The branches $\epsilon_\pm(p_\perp, 0)$ correspond to the spectrum of a homogeneous ferroelectric $\epsilon_\pm(p_\perp, p_z)$ for $p_z = 0$. The solid line represents the doubly degenerate null mode, $\epsilon_0 = \Delta_1$, which is restricted in the momentum space within the range $0 < p_\perp < \Delta$.

where

$$\hat{W}(z) = \Delta_2(z) + [\mathbf{p}_\perp \times \vec{\sigma}_\perp]_z , \tag{4}$$

and $[\ldots]_z$ is the z component of the vector product. Quadrating matrix (3), we obtain the Hamiltonian of supersymmetric quantum mechanics[3]

$$\hat{H}^2 = \hat{p}_z^2 + \hat{W}^2(z) + \hbar v_\parallel \hat{W}'(z) \otimes \hat{\tau}_z + \Delta_1^2 . \tag{5}$$

The operators $\hat{H}^2_\pm$ in (5) correspond to two values $\tau_z = \pm 1$. We know[3] that, with the exception of the ground state (null mode), the eigenvalues of these operators are the same, $\epsilon_0^2 = \Delta_1^2$. A null mode exists when the asymptotic expressions of the eigenvalues of the operator of superpotential (4)

$$W^\pm(z) = \Delta_2(z) \pm p_\perp \tag{6}$$

have opposite signs in the limit $z \to \pm\infty$. If $W^\pm(+\infty) > 0$ and $W^\pm(-\infty) < 0$, the energy of this mode is $\epsilon_0 = +\Delta_1$ (Fig. 1). In this case the lower spinor component of the eigenfunction of Hamiltonian (3) is $\psi_+ = 0$ and the upper component ψ_- satisfies the equation

$$(i\hat{p}_z + \hat{W}(z))\,\psi_- = 0. \tag{7}$$

For different signs of the asymptotic expressions $\epsilon_0 = -\Delta_1$ and $\psi_- = 0$, and only the ψ_+ function is normalizable. The null mode thus splits off from the conduction band or the valence band, depending on the sign of the charge of the domain wall and the sign of Δ_1, i.e., on whether the terms at the L points of the paraelectric phase are inverted (as they are in SnTe but are not in PbTe).

Two linearly independent solutions of Eqs. (7) are

$$\psi^{(\pm)} = \frac{C}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm(k_y + ik_x)/k_\perp \end{pmatrix} \exp\left[-\frac{1}{\hbar v_\parallel}\int_0^z W^\pm(z)dz\right]. \tag{8}$$

If $\Delta_2(\pm\infty) = \pm\Delta$ and $\Delta > 0$, these solutions are normalizable only at $p_\perp < \Delta$. The null mode is therefore doubly degenerate and is restricted in the momentum space (Fig. 1). These properties are attributable to only the supersymmetry and global properties of the potential of the inverse domain wall[2] $\Delta_2(z)$.

For the standard dependence

$$\Delta_2(z) = \Delta \tan(z/l) \tag{9}$$

the coordinate part of the wave function (8) is

$$f^\pm(z) = C\exp\left(\pm\frac{p_\perp z}{\Delta l_\parallel}\right)\cosh^{-l/l_\parallel}(z/l). \tag{10}$$

The length $l_\parallel = \hbar v_\parallel/\Delta$ for $\Delta \sim 30$ meV ($Pb_{0.9}Ge_{0.1}Te$ at[1] $T = 0$ K) and $v_\parallel \sim 3\times 10^7$ cm/s is on the order of 100 Å. Since this value does not exceed the normal thickness of the domain wall, the null mode is the only discrete level in the spectrum of the Hamiltonian $\hat{H}^2_-$. For $l > l_\parallel$, there can be other states which are localized at the domain wall.[4] Not being supersymmetric, these states are not degenerate and their energy depends on $p_\perp$. The number of states in the null mode per unit area, $N_0 = (2\pi l_\perp^2)^{-1}$, is determined by the "transverse" length $l_\perp = \hbar v_\perp/\Delta$. At $v_\perp \sim 10^8$ cm/s, $l_\perp \sim 300$ Å and $N_0 \sim 10^{10}$ cm^{-2}.

In contrast with the null mode, the energies of delocalized states corresponding to the superpotentials $W^\pm$ may be different. The Schrödinger equations for them are

$$(\hat{p}_z^2 + \Delta_2^2(z) + \hbar v_\parallel \Delta'_2(z) + p_\perp^2 + \Delta_1^2 \pm 2p_\perp\Delta_2(z) - \epsilon^2)\psi_+^{(\pm)} = 0. \tag{11}$$

Although in the inverse contract[4] a potential like that in (9) gives rise to a reflectionless situation, here the carriers with a constant $p_\perp$ and with an energy ϵ, enclosed in the interval $\epsilon_-(p_\perp, 0) < \epsilon < \epsilon_+(p_\perp, 0)$ between the branches of a continuous spectrum (Fig. 1), cannot pass through a domain wall because of the term $\pm 2p_\perp\Delta_2(z)$. In a system of domains the energy $\tilde{\Delta} = (\Delta_1^2 + \Delta^2)^{1/2}$ is therefore the mobility threshold.

In the presence of a magnetic field H parallel to the z axis, we should make the substitution $\hat{p}_\perp \to (\hat{p}_x, \hat{p}_y - x\hbar v_\perp/L^2)$ in the operator $\hat{W}(z)$, where $L^2 = \cos \hbar/eH$. The eigenvalues of such a superpotential are

$$W^\pm(z) = \Delta_2(z) \pm \sqrt{2n}\,\hbar v_\perp/L; \quad n = 0, 1, 2, \ldots. \tag{12}$$

Because of the supersymmetry, all states with $n < n_m$, for which the alternating signs of $W^\pm(z)$ remain in force, have identical energy, $\epsilon_0 = \Delta_1$. The maximum value of n is $n_m = [L^2/2l_\perp^2]$, where the brackets denote the integral part. The degeneracy of the state with $n = 0$ is $N_L = 1/2\pi L^2$ and that of the other states in $2N_L$. The total number of states in the null mode is $N_0(H) = N_L(1 + 2n_m)$. For integral values $n = L^2/2l_\perp^2$ the quantity $N_0(H)$ changes spasmodically from $N_0(1 - 1/2n)$ to $N_0(1 + 1/2n)$, hy-

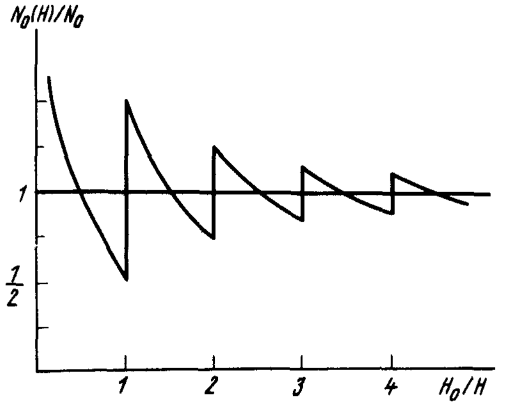

FIG. 2. Quantum oscillations of the states in the null mode in an external magnetic field H. The variation scale of the field is $H_0 = \Phi_0/4\pi l_1^2 \sim 10^4$ G.

perbolically tending to N_0 in the limit $H \to 0$. The abrupt changes in $N_0(H)$ correspond to the magnetic field $H_n = \Phi_0/4\pi l_1^2 n$, where $\Phi_0 = 2\pi\hbar c/e$ is a fluxoid (Fig. 2).

We should point out in conclusion that the presence of a state-density peak in the spectrum (Fig. 1) should lead to appreciable collective effects similar to those observed in systems with heavy fermions or to a condensation of the gas-liquid type in the null mode.

[1)]Since the electric field of such a domain wall is relatively small ($\sim 10^3$ V/cm), a potential drop of ~ 1 meV along the scale length $l_\parallel \sim 100$ Å (more on this point below) can be ignored.
[2)]We see that a null mode exists even at neutral (110) domain walls. This mode, which is attributable to crystalline anisotropy, can occur for two L valleys [− 1, 1, 1] and [1, − 1, 1] which do not lie in the plane of the domain wall.

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