Semimetallic properties of a heterojunction

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(Submitted 16 July 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 5, 207–210 (10 September 1985)

The effect of fluctuations of the components of a solid solution on the properties of a junction of two semiconductors with an inverted band structure is studied. At least one of the semiconductors is considered to be semimagnetic. The specific heat and conductivity of the heterojunction are calculated.

We consider a junction between two semiconductors with an inverted band structure (the valence band of one of the semiconductors transforms in accordance with the same irreducible representation of the symmetry group as the conduction band of the other semiconductor, and vice versa). Such junctions are formed, for example, by compounds belonging to the lead, europium, MnTe, HgSe, CdTe, etc. chalcogenide group. Volkov and Pankratov[1] have shown that a contact of this sort is a potential well for longitudinal motion. The charge carriers captured by the potential well form a 2D layer. The spectrum of this layer consists of several branches, among which there is even a gap-free branch.

We will show below that the presence of a gap-free mode accounts for the metallic behavior of the contact, despite the presence in it of magnetic inhomogeneities.

We describe a heterojunction as a 2D solid solution with fluctuations in the concentration of the components. In the effective-mass approximation, a contact of this sort is described in Kane's model by a Hamiltonian (see Refs. 1 and 2, for example), in which the width of the energy gap $E_g(z)$ is a function of the z coordinate

$$\hat{H} = \hat{H}_0 + v_\perp \hat{\tau}^1 \otimes (p_x \hat{\sigma}^1 + p_y \hat{\sigma}^2) + \hat{V}(x, y) \tag{1}$$

$$H_0 = E_g(z) \hat{\tau}^3 \otimes \hat{I}_\sigma - i v_\parallel \frac{\partial}{\partial z} \hat{\tau}^1 \otimes \hat{\sigma}^3 \,. \tag{2}$$

$\hat{H}$ operates in the vector space $\Psi_\sigma^{(\tau)}(\sigma = \pm 1/2,\ \tau = \pm 1)$, where σ are the spin indices, τ are the (valence and conduction) band indices, $\hat{\tau}^i$ and $\hat{\sigma}^i$ are the Pauli matrices which act in the appropriate subspace, and $\hat{I}$ is a unit matrix. The term $\hat{V}(x, y)$ describes the inhomogeneity of the contact. $E_g(\pm\infty) = \pm E$, and because of the symmetry, the chemical potential lies in the middle of the band gap, an important factor in our discussion below.

If $E_g(z) = E_g = \text{const}$, the spectrum of Hamiltonians (1) and (2) will be

$$\epsilon^2 = E_g^2 + v_\parallel^2 p_z^2 + v_\perp^2 (p_x^2 + p_y^2).$$

Such a model describes well the spectrum of ternary compounds of the type[2] $Pb_{1-c}Sb_cTe$ near the Brillouin zone where the energy gap has a minimum.

Assuming that $E_g(z)$ is a reasonably strong function and following the procedure used in Ref. 1, we will diagonalize the longitudinal part of the Hamiltonian specified

by expression (2), while treating the transverse motion as though it were a perturbation. The spectrum of H_0 is a discrete spectrum which includes the normalizable mode with a zero-point energy:

$$\Psi_\sigma^{(\tau)}(x, y, z) = f_\sigma^{(x, y)} \exp(-\rho(z)) \frac{1}{\sqrt{2}} \begin{pmatrix} -i\sigma \\ 1 \end{pmatrix} \tag{3}$$

$$\rho(z) = v_\parallel^{-1} \int_0^z E_g(z')\, dz' .$$

We assume that $E_1 \sim v_\parallel / d$ (d is the width of the contact) is the first nonzero eigenvalue of Hamiltonian (2); at small transverse momenta $p_\perp \ll E_1 / v_\perp$, the perturbation of function (3) by the virtual transitions to the nonzero levels of Hamiltonian (2) may be disregarded. In the basis of function (3) the transverse-motion Hamiltonian is

$$H = v_\perp (\hat{\sigma}^2 p_x + \hat{\sigma}^1 p_y) + \hat{\sigma}^3 V(x, y) . \tag{4}$$

It is easy to see that of all possible perturbations $V(x, y)$, only the perturbations with the structures $\hat{I}_\tau \otimes \hat{I}_\sigma$ and $\hat{I}_\tau \otimes \sigma_3$ have a nonzero projection on the basis of (3). The first structure corresponds to fluctuations of the chemical potential—because these fluctuations are small, we will not consider them here. The second structure, a random magnetic field, arises if the contact includes magnetic semiconductors. A perturbation of this sort is included in Eq. (4)

$$V(x, y) = \frac{dA}{dc} \frac{1}{n_0} \int \exp(-2\rho(z)) \delta n(\mathbf{r}) dz \;/\; \int \exp(-2\rho(z')) dz' , \tag{5}$$

where δn is a fluctuation of the density of magnetic atoms, n_0 is the total density, c is the index of the fraction of magnetic atoms, and A is the constant of the exchange interaction of the electrons with the atoms of the solution. In the Gaussian approximation, the probability $W(\delta n)$ for a change in the density δn is

$$W(\delta n) = \exp\left(- \int \frac{\delta n^2(x, y, z) d^3 r}{2 n_0 c (1 - c)} \right). \tag{6}$$

Therefore, we have

$$< V(x, y)\, V(x', y') > = g_0\, \delta(x - x') \delta(y - y') ,$$

$$g_0 = \frac{c(1-c)}{4 n_0 v_\perp^2} \left(\frac{dA}{dc} \right)^2 \int \exp(-4\rho(z))\, dz \;/\; \left(\int \exp(-2\rho(z')) dz' \right)^2 . \tag{7}$$

Since the impurity potential is a static potential, we can consider single-electron Green's functions at the given frequency:

$$G(\omega) = (i\omega - \hat{H})^{-1} .$$

Averaging over the impurities reduces to a 2D Euclidean field theory with the Lagrangian

$$L = i \bar{\Psi}_n \gamma_\mu \partial_\mu \Psi_n - i\omega \bar{\Psi}_n \gamma_5 \Psi_n + g_0 (\bar{\Psi}_n \Psi_n)^2 , \tag{8}$$

where $n = 1,...,N$; in the final result we must set $N = 0$. The renormalization-group equations for theory (8) were derived in Ref. 3. According to the approach in Ref. 3, the elementary vertex g_0 is renormalized:

$$g(\xi) = g_0\left(1 + \frac{g_0}{\pi}\ln\frac{\Lambda}{|\xi|}\right)^{-1}, \qquad \begin{array}{l}\Lambda \sim |E_1|\\ \xi = max(\omega, v_\perp p)\end{array} \tag{9}$$

Consequently, the effective interaction of the charge carriers with the impurities falls off at low energies (momenta); the perturbation theory becomes progressively more effective as the energy is reduced. We see from (9) that the renormalization of the vertex is appreciable at $|\xi| \lesssim \Lambda \exp(-\pi/g_0)$, where $g_0 \ln(\Lambda/|\xi|) \gtrsim 1$.

The average Green's function is

$$\hat{G}(\omega, p) = -(\omega^2\Sigma^2(\xi) + p^2v_\perp^2)^{-1}(i\omega\hat{I} + p\hat{\sigma}), \tag{10}$$

$$\Sigma^2(\xi) = \left(1 + \frac{g_0}{\pi}\ln\Lambda/|\xi|\right).$$

The state density is

$$\rho(\epsilon) = \frac{1}{4\pi^3}\mathrm{Im}\int d^2p\,\mathrm{Sp}\hat{G}^R(\epsilon, p) = \frac{1}{2v_\perp^2}|\epsilon|\Sigma(\epsilon) \tag{11}$$

and the specific heat is

$$c_v \sim T^2\Sigma(T) \sim T^2\left(1 + \frac{g_0}{\pi}\ln\frac{\Lambda}{T}\right)^{1/2}. \tag{12}$$

Analysis of the diagram theories for the conductivity shows that the Drude equation

$$\sigma = \frac{e^2}{4\pi}\frac{|\Sigma^R(\epsilon)|^2}{\mathrm{Im}(\Sigma^R(\epsilon))^2} = \frac{e^2}{4\pi}\left(\frac{1}{g_0} + \frac{1}{\pi}\ln\frac{\Lambda}{T}\right) \tag{13}$$

can be used to calculate σ. The corrections to this formula contain relatively small terms, $\sim g(T)\ln[1/g(T)]$.

The equations we derived here differ from the equations in the Born approximation in that g_0 is replaced by $g(T)$, the total scattering amplitude.

We thus see that the conductivity tends toward infinity in a logarithmic manner as $T \to 0$! The effect of impurities, which is seen in normal metals as a residual resistance and in 2D systems with a finite Fermi surface as a total localization of charge carriers, disappears in this case. The electrons with energies $\epsilon \sim T$ participate in the conductivity. In normal metals, such electrons have large momenta, $p \approx p_F \sim \pi/a$ (a is the lattice constant). In our case, on the other hand, $\epsilon = pv_\perp$, the Fermi momentum is $p_F = 0$, and the characteristic wavelength of the charge carriers increases with decreasing temperature, $\lambda \sim 1/T$. The electrons with longer wavelengths of course are scattered more weakly by the inhomogeneities of the potential. We see from (13) that the mean free path increases logarithmically: $l \sim 1/\ln(\Lambda/T)$.

We wish to thank É. I. Rashba and A. S. Ioselevich for useful discussions. We also thank S. I. Gubarev for furnishing his experimental results.

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Translated by S. J. Amoretty