THEORY OF UNIAXIAL CRYSTALS WITH ZERO FORBIDDEN BAND

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The effect of Coulomb interaction between electrons in a gapless semiconductor is estimated. The case of a strongly anisotropic semiconductor is considered. The dispersion law is given by expression (A). It is demonstrated that in contrast to the familiar case of an isotropic dispersion law, the logarithmic approximation remains valid for renormalizations of all quantities, and only the interaction along the z-axis changes significantly.

1. INTRODUCTION

As shown by Abrikosov and Beneslavskiĭ [1], crystal symmetry admits of the possibility of contact between the valence band and the conduction band. Indications of the possible existence of substances with such properties appeared recently in the literature (grey tin [2] and mercury telluride [3]). Obviously, at sufficiently low temperatures the main type of interaction will be the Coulomb interaction between the electrons. Abrikosov and Beneslavskiĭ [1] took into account the interelectron interaction for two types of spectra in the vicinity of the point of contact between the bands: linear-isotropic and quadratic-isotropic. It was shown that the role of the Coulomb interaction in these two cases is entirely different. It was therefore of interest to investigate the intermediate case when an unisotropic dispersion law.

We consider here a model with a linear dependence of the energy on the quasimomentum along the crystal axis and a quadratic dependence in the basal plane. Thus, in the absence of interaction, the energy spectrum is determined as follows [1]:

$$\varepsilon_{1,2} = \alpha k_\perp^2 + \gamma k_z^2 \pm (\beta^2 k_z^2 + \xi^2 k_\perp^4)^{1/2},$$

where α, β, γ, and ξ are constants and $k_\perp^2 = k_x^2 + k_y^2$. A spectrum of this type is possessed by crystals with a symmetry corresponding to the point groups D_3 and D_6. It can be shown that examination of a more general case with a dispersion law corresponding to any group D_n does not lead to any qualitatively new results.

Since the most interesting region is the vicinity of the point of contact between the bands, i.e., the region of small momenta on the equal-energy surface where the relation

$$\gamma k_z^2 \sim \gamma\left(\frac{\xi}{\beta} k_\perp^2\right)^2 \ll \alpha k_\perp^2$$

is satisfied, the energy spectrum becomes simpler:

$$\varepsilon_{1,2} = \alpha k_\perp^2 \pm (\beta^2 k_z^2 + \xi^2 k_\perp^4)^{1/2}. \tag{A}$$

We assume, for simplicity, that the spin-orbit interaction is small and can be neglected.

It must be emphasized that the energy spectrum of real crystal (HgTe and α-Sn) is more complicated than that considered by us. Nonetheless, such a problem is not only of methodological interest, since a spectrum of type (A) can be realized, for example, in alloys or under pressure.

2. FIRST PERTURBATION-THEORY CORRECTIONS

The Green's function for non-interacting electrons can be written in the form [4]

$$\hat{G}_0^{-1} = \omega - \alpha k_\perp^2 - \hat{Q} + i\delta \operatorname{sign}\omega,$$
$$\hat{Q} = \sigma_x \xi (k_x^2 - k_y^2) + 2\sigma_y \xi k_x k_y + \sigma_z \beta k_z. \tag{1}$$

We introduce the Coulomb interaction between the electrons and examine how the screening takes place. The screened interaction is of the form

$$D(\mathbf{q}, \omega) = \frac{4\pi e^2}{\varepsilon_z^{(0)} q_z^2 + \varepsilon_\perp^{(0)} q_\perp^2 - 4\pi e^2 \Pi(\mathbf{q}, \omega)}, \tag{2}$$

where $\Pi(q, \omega)$ is the sum of all possible electron loops. In the first approximation

$$\Pi(\mathbf{q}, \omega) = -i \operatorname{Sp} \int \hat{G}_0(\omega_1; \mathbf{k}) \hat{G}_0(\omega + \omega_1; \mathbf{k} + \mathbf{q}) \frac{d\omega_1 d^3k}{(2\pi)^4}. \tag{3}$$

Integrating in (3) with respect to the internal frequencies and taking the trace, we obtain

$$\Pi(\omega, q) = \Pi_+(\omega, \mathbf{q}) + \Pi_-(\omega, \mathbf{q}), \quad \Pi_+(\omega, q) = \Pi_-(-\omega, \mathbf{q}), \tag{4}$$

where

$$\Pi_+(\omega, \mathbf{q}) = \int \frac{Q_1 Q_2 - |Q_1||Q_2|}{4|Q_1||Q_2|} \frac{1}{\omega + \alpha[k_\perp^{(1)2} - k_\perp^{(2)2}] + |Q_1| + |Q_2|} \cdot \frac{d^3k}{(2\pi)^3};$$
$$\hat{Q}_1 = Q(\mathbf{k}), \ \hat{Q}_2 = \hat{Q}(\mathbf{k}+\mathbf{q}); \quad \mathbf{k}_\perp^{(1)} = \mathbf{k}_\perp, \ \mathbf{k}_\perp^{(2)} = \mathbf{k}_\perp + \mathbf{q}_\perp. \tag{5}$$

Expressions (4) and (5) contain corrections to $\epsilon_\perp$ and ϵ_z. It is therefore more convenient to break up Π into two parts:

$$\Pi = \Pi_\perp + \Pi_z = q_\perp^2 \delta\varepsilon_\perp + q_z^2 \delta\varepsilon_z. \tag{6}$$

We consider first the expression for $\delta\epsilon_\perp$. We put for simplicity $q_Z = 0$. Since the largest contribution to the integral in (5) for $\delta\epsilon_\perp$ is made by the region of the internal variables, which are much larger than the external ones, i.e., $q_\perp^2 \ll k_\perp^2 \sim \beta k_Z/\xi \gg \beta q_Z/\xi$, we can expand with respect to $q_\perp/k_\perp$. Accurate to third-order terms, we obtain

$$|Q_1||Q_2| - \mathbf{Q}_1\mathbf{Q}_2 = \tfrac{1}{2}|Q|^{-2}\{4\xi^4[k_\perp^6 q_\perp^2 - (\mathbf{k}_\perp\mathbf{q}_\perp)^2 k_\perp^4] + 4\xi^2\beta^2 k_\perp^2 k_z^2 q_\perp^2\}. \tag{7}$$

Substituting (7) in (5), we obtain, with logarithmic accuracy,

$$\delta\varepsilon_\perp = \frac{1}{3\pi}\frac{e^2}{\beta}\ln\frac{q}{L}, \tag{8}$$

where $q = \max(q_z, \xi q_\perp^2/\beta, \omega/\beta)$, and L is the cutoff momentum. Consequently, along the xy plane the Coulomb interaction is practically not screened.

We consider now the expression for $\delta\epsilon_z$. We put for simplicity $q_\perp = 0$. No expansion is possible for $\delta\epsilon_z$. Exact calculation of (5) yields

$$\Pi_z = \frac{1}{48\pi^2}\frac{1}{\xi} q_z \frac{\beta q_z}{(\beta^2 q_z^2 - \omega^2)^{1/2}}. \tag{9}$$

Substituting (8) and (9) in (2), we obtain

$$D(\mathbf{q},\omega) = 4\pi e^2 \left[q_\perp^2 \varepsilon_\perp^{(0)} \left(1 + \frac{1}{3\pi}\frac{e^2}{\varepsilon_\perp^{(0)}\beta} \ln\frac{q}{L}\right) \right. \tag{10}$$

$$\left. + \varepsilon_z^{(0)} q_z^2 + \frac{1}{12\pi}\frac{e^2}{\xi} q_z \frac{\beta q_z}{(\beta^2 q_z^2 - \omega^2)^{1/2}} \right]^{-1}.$$

It is seen from (10) that the region of permissible values of q_Z can be naturally broken up into the following three subregions:

I. Region of large momenta

$$\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L} \ll 1, \quad q_z \gg \frac{e^2}{\varepsilon_z^{(0)}\xi}.$$

II. Region of small momenta

$$\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L} \ll 1, \quad q_z \ll \frac{e^2}{\varepsilon_z^{(0)}\xi}.$$

III. Region of ultrasmall momenta

$$\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L} \gg 1, \quad q_z \ll \frac{e^2}{\varepsilon_z^{(0)}\xi}.$$

In the region of large momenta, perturbation theory is valid and all the corrections are small.

3. REGIONS OF SMALL AND ULTRASMALL MOMENTA

We consider first the region II. We shall show that for this region it suffices to take into account in (2) only the simplest electron loop, and all the remaining terms yield small corrections. We consider to this end a vertex with one Coulomb line:

$$\delta\Gamma(\omega;\mathbf{k},\mathbf{q}) = \int \hat{G}(\omega-\omega_1;\ \mathbf{k}-\mathbf{k}^{(1)})\hat{G}(\omega-\omega_1+\omega_q;\mathbf{k}-\mathbf{k}^{(1)}+q) \times D(\mathbf{k}^{(1)})\frac{d^3k^{(1)}d\omega_1}{(2\pi)^4}. \tag{11}$$

For simplicity we can consider only the scalar part of (11), i.e., an integral of the form

$$\delta\Gamma_{\text{ск}} = \int \frac{Q_1Q_2 - |Q_1||Q_2|}{4|Q_1||Q_2|} \frac{D(\mathbf{k}^{(1)})}{\omega + a(k_\perp^{(1)2} - k_\perp^{(2)2}) + |Q_1| + |Q_2|}\frac{d^3k^{(1)}}{(2\pi)^3};$$

$$Q_1 = Q(\mathbf{k}-\mathbf{k}^{(1)}), \quad Q_2 = Q(\mathbf{k}-\mathbf{k}^{(1)}+\mathbf{q}). \tag{12}$$

It can be shown that the discarded terms are of the same order.

We note that the main contribution in (12) after integration with respect to $k_\perp^{(1)}$ is made by the region in which the internal variables are close to the external ones, i.e., the region of small $k_\perp^{(1)}$. In what follows, we shall need on several occasions to estimate integrals of the type

$$I(\mathbf{k}) = \int F(\mathbf{k};k_\perp',k_z')D(k_\perp',k_z')d^2k_\perp'dk_z', \tag{13}$$

where $F(k, k_\perp', k_Z')$ is a sufficiently smooth function of all the arguments. As will be shown below, in the principal region it can be assumed that $F(\mathbf{k}; k_\perp', k_Z') = F(\mathbf{k}; 0, k_Z')$. Consequently, integration with respect to $k_\perp'$ affects only the function D. With logarithmic accuracy, we obtain

$$I(\mathbf{k}) = \int F(\mathbf{k};0,k_z')D(k_\perp',k_z')d^2k_\perp'dk_z'$$

$$= \int F(\mathbf{k};0,k_z')\frac{4\pi e^2}{\varepsilon_\perp k_\perp'^2 + c_1 e^2 k_z'} d^2k_\perp'dk_z' \tag{14a}$$

$$= \int F(\mathbf{k};0,k_z')\frac{4\pi e^2}{\varepsilon_\perp}\ln\frac{\varepsilon_\perp k_{\perp\,max}^2}{c_1e^2k_z'}dk_z' = \int F(\mathbf{k};0,k_z')\bar{D}(k_z')dk_z',$$

where

$$\frac{1}{\beta}\bar{D}(k_z) = \frac{1}{\beta}\frac{4\pi e^2}{\varepsilon_\perp}\ln\frac{\varepsilon_\perp k_{\perp\,max}^2}{c_1e^2k_z} \sim \tag{14b}$$

$$\sim \frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln\frac{\varepsilon_\perp^{(0)}k_{\perp\,max}^2}{c_1e^2k_z}\left(1+\frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln\frac{k_z}{L}\right)^{-1} \ll 1$$

and $c_1 = 1/12\pi\xi$. The quantity $\tilde{D}(k_Z)$ characterizes the interaction forces along the axis. All the diagrams will contain integrals of the type (13), which can be reduced to expressions of the type (14). We now consider in greater detail the first correction (12) to the vertex part.

Since $k_\perp' = 0$ in the region of interest to us, the integrand can be rewritten in the form

$$\frac{|Q_1||Q_2| - Q_1Q_2}{2|Q_1||Q_2|} = \frac{|k_z'||k_z'-q_z| - k_z'(k_z'-q_z)}{2|k_z'||k_z'-q_z|} = \begin{cases} 0, & k_z' > q_z \\ 1, & 0 < k_z' < q_z \\ 0, & k_z' < 0 \end{cases} \tag{15}$$

We have put for simplicity $k_\perp' = q_\perp' = 0$, which does not change the order of magnitude, as can be readily verified. Substituting (15) in (12), we obtain

$$\delta\Gamma_{\text{sc}} \approx \int_0^{q_z} \frac{dk_z}{\omega - \beta q_z}\bar{D}(k_z) \sim \frac{1}{\beta}\bar{D}(q_z) \ll 1. \tag{16}$$

Obviously, the higher-order corrections will contain $(\tilde{D}/\beta)^n \ll 1$. Consequently, the corrections to the vertex can be neglected.

We now consider the energy-spectrum renormalization connected with allowance for the Coulomb interaction. We estimate the first term in the expression for the self-energy part

$$\delta\hat{\Sigma}(\omega;\mathbf{q}) = i\int \hat{G}(\omega';\mathbf{k})D(\omega-\omega';\mathbf{q}-\mathbf{k})\frac{d^3kd\omega'}{(2\pi)^4}. \tag{17}$$

Integrating in (17) with respect to the frequency, we obtain

$$\delta\hat{\Sigma} = \int \frac{|Q|+\hat{Q}}{2|Q|}D(\mathbf{q}-\mathbf{k})\frac{d^3k}{(2\pi)^3}. \tag{18}$$

We consider first the influence of the Coulomb interaction on the renormalization of β and ξ. In (18), this corresponds to a term of the type

$$\delta\hat{\Sigma} = \int \frac{\hat{Q}}{2|Q|}D(\mathbf{q}-\mathbf{k})\frac{d^3k}{(2\pi)^3}. \tag{18a}$$

To obtain the correct estimate, it is sufficient to consider any one of the components of $\delta\hat{\Sigma}$, for example $\delta\Sigma_X$:

$$\delta\Sigma_x = \int \frac{\xi(k_x^2-k_y^2)}{(\beta^2k_z^2+\xi^2k_\perp^4)^{1/2}}D(\mathbf{q}-\mathbf{k})\frac{d^3k}{(2\pi)^3}. \tag{19}$$

We calculate the integral by the same method as used for the integral in (14). We obtain

$$\delta\Sigma_x = \frac{q_x^2-q_y^2}{(2\pi)^3}\xi\int\frac{\bar{D}(q_z-k_z)}{(\beta^2k_z^2+\xi^2k_\perp^4)^{1/2}}dk_z. \tag{20}$$

The main contribution to the integral in (20) is made by the region

$$\varepsilon_\perp^{(0)}\xi q_\perp^2/e^2 \gg k_z \gg \xi q_\perp^2/\beta.$$

We obtain ultimately

$$\delta\Sigma_x = (q_x^2 - q_y^2)\Delta\xi = \frac{q_x^2-q_y^2}{(2\pi)^3}\frac{\xi_0}{\beta}\int\frac{dk_z}{k_z}\bar{D}(q_z-k_z)$$
$$= \frac{q_x^2-q_y^2}{4\pi^2}\xi_0\frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln^2\frac{\varepsilon_\perp^{(0)}\beta}{e^2}. \quad (21)$$

Consequently, the correction to ξ is equal to

$$\Delta\xi = \frac{1}{4\pi^2}\xi_0\frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln^2\frac{\varepsilon_\perp^{(0)}\beta}{e^2} \ll \xi_0. \quad (22)$$

Obviously, a similar correction arises for the remaining components of $\delta\hat{\Sigma}$. Thus, we have with logarithmic accuracy in the region of small momenta

$$\xi = \xi_0\left(1+\frac{1}{4\pi^2}\frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln^2\frac{\varepsilon_\perp^{(0)}\beta}{e^2}\right),$$

$$\beta = \beta_0\left(1+\frac{1}{4\pi^2}\frac{e^2}{\beta\varepsilon_\perp^{(0)}}\ln^2\frac{\varepsilon_\perp\beta}{e^2}\right),$$

$$\varepsilon_\perp = \varepsilon_\perp^{(0)}\left(1+\frac{1}{3\pi}\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L}\right).$$

We now find the corrections to α to allow for the Coulomb interaction. It is sufficient to confine ourselves in (18) to the expression

$$\Sigma = \int D(\mathbf{q}-\mathbf{k})d^3k. \quad (18b)$$

The integral in (18b) diverges formally. To eliminate the divergence we can, as is well known, calculate in place of $\Sigma(\omega, \mathbf{q})$ the difference $\Sigma(\omega, \mathbf{q}) - \Sigma(0, 0)$. This yields, in order of magnitude,

$$\alpha = \alpha_0[1 + ef(q_z/q_\perp)],$$

where $f(q_z/q_\perp)$ is a function of the order of unity.

We consider now the region of ultrasmall momenta. We shall show first that here, as in the preceding case, it suffices to take into account only the simplest loop. To prove this, we consider the first-order corrections to the vertex. Transforming the general expression (12) into (14) and taking (15) into account, we obtain

$$\delta\Gamma \approx \int_0^{q_z}\frac{dk_z}{\omega-\beta|k_z|-\beta|k_z-q_z|}\bar{D}(q_z-k_z) \sim \frac{1}{\beta}\bar{D}(q_z) \ll 1. \quad (23)$$

This result, of course, is to be expected, for when q_z decreases we come closer and closer to the "Fermi point," i.e., to the point of contact between the valence and the conduction bands. Therefore the dielectric constant can increase in comparison with the value for the region where the bands are far from each other. This is precisely reflected in (14b) and in the estimate (23).

We consider now the renormalization of the energy spectra. Just as in the region of small momenta, it is sufficient to estimate only any one component of $\delta\Sigma$, say $\delta\Sigma_x$. The expression (20) remains valid:

$$\delta\Sigma_x = \frac{q_x^2-q_y^2}{(2\pi)^3}\xi_0\int\frac{dk_z}{(\beta^2k_z^2+\xi^2k_\perp^4)^{1/2}}\frac{4\pi e^2}{\varepsilon_\perp}\ln\frac{\varepsilon_\perp k_{\perp max}^2}{c_1e^2k_z}. \quad (24)$$

Substituting

$$\varepsilon_\perp = \varepsilon_\perp^{(0)}\left[1+\frac{1}{3\pi}\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L}\right],$$

we obtain from (24)

$$\Delta\xi = \xi_0\frac{1}{4\pi^2}\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\left(1+\frac{1}{3\pi}\frac{e^2}{\varepsilon_\perp^{(0)}\beta}\ln\frac{q}{L}\right)^{-1}\ln^2\frac{\varepsilon_\perp^{(0)}\beta}{e^2} \ll \xi_0. \quad (25)$$

Obviously, a similar estimate is valid for $\Delta\beta$. Thus, in all three regions, owing to the smallness of the effective interaction, the renormalization of the spectrum is small. The Coulomb potential is practically unscreened in the xy plane. Along the z axis, the interaction changes significantly.

In conclusion we wish to call attention to the dependence of the dielectric constant on the momentum (formulas (8) and (9)). We see that $\epsilon_\perp$ varies little, whereas $\epsilon_z \to \infty$ as $q \to 0$. Such a situation is absolutely untypical for the previously known substances and can become manifest only in strongly unisotropic crystals with zero forbidden band.

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32