THRESHOLD PHENOMENA IN A GAPLESS SEMICONDUCTOR WITH A LINEAR SPECTRUM

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The effect of Coulomb interaction between electrons near the threshold is estimated. A gapless semiconductor with a linear isotropic dispersion law is considered. It is demonstrated that at small distances ahead of the threshold, motion in a plane perpendicular to the external momentum is quantized. Bound states arise which are similar to Landau levels.

1. INTRODUCTION

ABRIKOSOV and Beneslavskiĭ [1] advanced the hypothesis that gapless semiconductors exist, and investigated their properties. They have shown that in crystals with cubic symmetry and with symmetry corresponding to the groups D_n the electron spectrum is isotropic:

$$\omega = \pm vq. \tag{1}$$

The Green's function for the non-interacting electrons is[1]

$$\hat{G}_0 = [\omega - v\sigma\mathbf{q} + i\lambda\,\mathrm{sign}\,\omega]^{-1}, \quad \lambda \to +0. \tag{2}$$

The Coulomb interaction between the electrons alters the Green's function little, and the resulting corrections are $\sim e^2 \ln(k_{max}/k)$, where k_{max} is of the order of the period of the reciprocal lattice, and are significant only in the region of exponentially small momenta. For the polarization operator that characterizes the interaction of the crystal with the external field, however, the Coulomb interaction is more significant. We shall show that these corrections are most appreciable near the two-electron threshold. In this region, the Coulomb interaction leads not to logarithmic but to power-law corrections of the type $e^2/\sqrt{vq - \omega}$. Summing the principal diagrams, we can find the character of the singularity of the polarization operator. It turns out here that at small distances there appear ahead of the threshold certain peculiar bound states in which the motion is quantized in a plane perpendicular to the momentum, in analogy with the Landau levels.

2. FIRST PERTURBATION-THEORY CORRECTIONS

In the absence of Coulomb interaction, the polarization operator (the diagram in Fig. 1a) is equal to

$$\Pi^{(0)} = -i\,\mathrm{Sp}\int \hat{G}_0(\omega - \omega_1; \mathbf{q} - \mathbf{k})\hat{G}_0(\omega_1; \mathbf{k})\frac{d\omega_1\, d^3k}{(2\pi)^4}. \tag{3}$$

Substituting the Green's function (2), we obtain

$$\Pi^{(0)} = \int \frac{|\mathbf{k}|\,|\mathbf{q}-\mathbf{k}| + \mathbf{k}(\mathbf{q}-\mathbf{k})}{2|\mathbf{k}|\,|\mathbf{q}-\mathbf{k}|}\,\frac{|\mathbf{k}| + |\mathbf{q}-\mathbf{k}|}{\omega^2 - v^2(|\mathbf{k}| + |\mathbf{q}-\mathbf{k}|)^2}\,\frac{d^3k}{(2\pi)^3} = -\frac{q^2}{12\pi^2 v}\ln\frac{q_{max}}{\sqrt{q^2 - \omega^2/v^2}}, \tag{4}$$

where q_{max} is an integration limit of the order of the period of the reciprocal lattice.

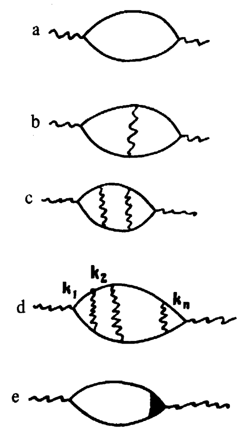


FIG. 1

Near the threshold ($\omega = qv$), this expression becomes infinite. In the integral (4), the following region of momenta is significant:

$$0 < k_z < q, \quad k_\perp \sim q\sqrt{\delta}, \tag{5}$$

where $\delta = (qv - \omega)/qv$ is the distance to the threshold, and the z axis is directed along q. The large contribution is due to the relatively broad region with respect to k_z.

We now take into account the Coulomb interaction. The first correction is determined by the diagram of Fig. 1b:

$$\Pi^{(1)} = -i\,\mathrm{Sp}\int \hat{G}(\omega_1; \mathbf{k}_1)\hat{G}(\omega_2; \mathbf{k}_2) \times \hat{G}(\omega - \omega_2; \mathbf{q} - \mathbf{k}_2)\hat{G}(\omega - \omega_1; \mathbf{q} - \mathbf{k}_1) \times D(\mathbf{k}_1 - \mathbf{k}_2)\frac{d\omega_1\, d^3k_1\, d\omega_2\, d^3k_2}{(2\pi)^4(2\pi)^4}. \tag{6}$$

Just as in (4), the largest contribution to (6) is made by the region where $k_{1,2}$ satisfied the inequality (5). In this region, the expression for the Green's function of the electron can be simplified:

$$\hat{G}(\mathbf{k}) = \frac{1}{\omega - v\hat{k}} = \frac{|\mathbf{k}| + \hat{k}}{2|\mathbf{k}|}\frac{1}{\omega - v|\mathbf{k}|} + \frac{|\mathbf{k}| - \hat{k}}{2|\mathbf{k}|}\frac{1}{\omega + v|\mathbf{k}|} \approx \frac{1+\sigma_z}{2}\frac{1}{\omega - v|\mathbf{k}|} + \frac{1-\sigma_z}{2}\frac{1}{\omega + v|\mathbf{k}|}, \tag{7}$$

$$\hat{k} = \sigma\mathbf{k}, \quad \mathbf{k} = (\mathbf{p}, \varkappa), \quad \mathbf{p} \parallel z, \quad \varkappa \perp z, \quad |\mathbf{k}| = p + \varkappa^2/2p.$$

The trace in (6) can now be taken in elementary fashion. Integrating with respect to the frequencies, we obtain

$$\Pi^{(1)} = -\frac{1}{4}\frac{1}{(2\pi)^6}\Big[\int\int\frac{e^2}{\varepsilon_0(\mathbf{k}_1-\mathbf{k}_2)^2}\frac{d^3k_1}{\omega - v(|\mathbf{k}_1|)+|\mathbf{q}-\mathbf{k}_1|)} \times \frac{d^3k_2}{\omega - v(|\mathbf{k}_2|+|\mathbf{q}-\mathbf{k}_2|)} - \int\frac{e^2}{\varepsilon_0(\mathbf{k}_1-\mathbf{k}_2)^2}\frac{d^3k_1}{-\omega - v(|\mathbf{k}_1|+|\mathbf{q}-\mathbf{k}_1|)} \times \frac{d^3k_2}{-\omega - v(|\mathbf{k}_2|+|\mathbf{q}-\mathbf{k}_2|)}\Big]. \tag{8}$$

The second term is negligible near the threshold. Further, we can integrate in (8) with respect to the difference $p_1 - p_2$, and only the Coulomb potential takes part in the integral. In the remaining factors, we can put $p_1 = p_2 \equiv p$, since the integral

$$\frac{e^2}{\varepsilon_0}\int\frac{d(p_1-p_2)}{(p_1-p_2)^2+(\varkappa_1-\varkappa_2)^2} = \frac{e^2}{\varepsilon_0}\frac{1}{|\varkappa_1-\varkappa_2|} \tag{9}$$

converges in the region $|p_1 - p_2| \sim |\kappa_1 - k_2| \sim q\sqrt{\delta}$.

As the result we obtain

$$\Pi^{(1)} = -\frac{1}{4}\frac{1}{(2\pi)^6}\frac{1}{q^2v^2}\int_0^q dp\frac{d^2\varkappa_1}{a(\varkappa_1)}\frac{d^2\varkappa_2}{a(\varkappa_2)}\frac{e^2}{\varepsilon_0|\varkappa_1-\varkappa_2|}, \tag{10}$$

$$a(\varkappa) = -\delta + \varkappa^2/2p(q-p).$$

Near the threshold, the expression (10) has a stronger singularity than (4):

$$\Pi^{(1)} \to \text{const}\cdot e^2\delta^{-1/2}. \tag{11}$$

Thus, the Coulomb interaction becomes appreciable at a distance $\delta \sim e^4$ to the threshold.

To find the polarization operator in the region $\delta \lesssim e^4$, it is necessary to sum corrections of higher order.

3. EQUATION FOR THE POLARIZATION OPERATOR

We separate the diagrams that make the largest contribution to the threshold region. It is natural to expect them to be the diagrams containing the largest number of intermediate two-electron states at a given power of e^2.

For example, the diagrams in Figs. 2a and 2b, which describe the production of several pairs, make a contribution $\sim(e^2\ln\delta)^2$, $e^4\delta^{-1/2}\ln\delta$, whereas the diagram of Fig. 1c

$$\Pi^{(2)} = -i\,\mathrm{Sp}\int\hat G(\omega_1;\mathbf{k}_1)\hat G(\omega_2;\mathbf{k}_2)\hat G(\omega_3;\mathbf{k}_3)\hat G(\omega-\omega_3;\mathbf{q}-\mathbf{k}_3) \times\hat G(\omega-\omega_2;\mathbf{q}-\mathbf{k}_2)\hat G(\omega-\omega_1;\mathbf{q}-\mathbf{k}_1)D(\mathbf{k}_1-\mathbf{k}_2)D(\mathbf{k}_2-\mathbf{k}_3)\frac{d^4k_1\,d^4k_2\,d^4k_3}{(2\pi)^4(2\pi)^4(2\pi)^4} \tag{12}$$

makes a contribution $\sim(e^2/\sqrt{\delta})^2$.

As a result we are left only with the diagrams $\pi(n)$ of the form in Fig. 1d, describing the Coulomb interaction of one electron-hole pair.

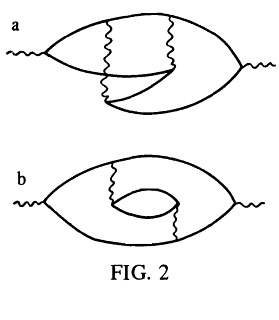
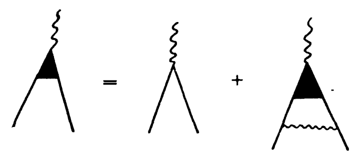


FIG. 2

For the sum of such diagrams (Fig. 1e) we can write the equation

$$\Pi = \sum_n \Pi^{(n)} = -i\,\mathrm{Sp}\int\hat G(\omega_1;\mathbf{k})\hat G(\omega-\omega_1;\mathbf{q}-\mathbf{k})\Gamma(\omega;\mathbf{q},\mathbf{k})\frac{d\omega_1\,d^3k}{(2\pi)^4}, \tag{13}$$

where the vertex part Γ satisfies the equation



(14)

In explicit form

$$\Gamma(\omega;\mathbf{q},\mathbf{k}) = 1 + \frac{1}{(2\pi)^4}\int\frac{e^2}{\varepsilon_0(\mathbf{k}-\mathbf{k}_1)^2}\frac{1}{\omega_1 - v\hat{k}_1}\Gamma(\omega;\mathbf{q},\mathbf{k}_1)\frac{d\omega_1\,d^3k_1}{\omega-\omega_1-v(\widehat{\mathbf{q}-\mathbf{k}_1})}. \tag{15}$$

It is easily seen that Γ does not depend on the electron frequency. We can therefore integrate with respect to ω_1 in (15):

$$\Gamma(\omega;\mathbf{q},\mathbf{k}) = 1 + \int\frac{e^2}{\varepsilon_0(\mathbf{k}-\mathbf{k}_1)^2}\Lambda_1\Gamma(\omega;\mathbf{q},\mathbf{k}_1) \cdot\Lambda_2\frac{1}{\omega - v(|\mathbf{k}_1|+|\mathbf{q}-\mathbf{k}_1|)}\frac{d^3k_1}{(2\pi)^3} + \int(\omega\to-\omega)d^3k, \tag{16}$$

$$\Lambda_1 = \frac{|\mathbf{k}_1|+\hat{\mathbf{k}}_1}{2|\mathbf{k}_1|},\quad \Lambda_2 = \frac{|\mathbf{q}-\mathbf{k}_1|+(\hat{\mathbf{q}}-\hat{\mathbf{k}}_1)}{2|\mathbf{q}-\mathbf{k}_1|}.$$

The term with the substitution $\omega\to-\omega$ in (16) is negligible near the threshold, and for the remaining term in (16), an important role will be played by the momentum region in which the projection operators Λ_1 and Λ_2 can be replaced by $(1+\sigma_z)/2$, and $|\mathbf{k}| = p + \kappa^2/2p$.

Further simplification results from the fact that the region $p - p_1 \sim q\sqrt{\delta}$ is important in (16) (p and p_1 are the longitudinal components of $\mathbf{k}$ and $\mathbf{k}_1$). Therefore only the Coulomb potential takes part in the integration, and in the remaining factors we can put $p = p_1$. As a result we get

$$\Gamma(\omega;\mathbf{q},\mathbf{k}) = 1 + \frac{1}{qv}\frac{1}{(2\pi)^3}\int\frac{e^2}{\varepsilon_0|\varkappa-\varkappa_1|} \times\Big[\frac{1+\sigma_z}{2}\Gamma(\omega;\mathbf{q},\mathbf{k}_1)\frac{1+\sigma_z}{2}\Big]\frac{d^2\varkappa_1}{a(\varkappa_1)}. \tag{17}$$

Similar simplifications in (13) yield

$$\Pi = \frac{1}{qv}\frac{1}{(2\pi)^3}\int dp\frac{d^2\varkappa}{a(\varkappa)}\mathrm{Sp}\Big[\frac{1+\sigma_z}{2}\Gamma\frac{1+\sigma_z}{2}\Big]. \tag{18}$$

These integral equations are solved in the next section.

4. SOLUTION OF THE EQUATION FOR Π

It is convenient to introduce a quantity $F(\mathbf{r}_\perp)$, which is connected with Γ in the following manner:

$$F(\mathbf{r}_\perp) = \int e^{i\varkappa\mathbf{r}_\perp}\frac{d^2\varkappa}{a(\varkappa)}\mathrm{Sp}\Big[\frac{1+\sigma_z}{2}\Gamma\frac{1+\sigma_z}{2}\Big]. \tag{19}$$

Then

$$\Pi = \frac{1}{qv}\frac{1}{(2\pi)^3}\int_0^q F(0)\,dp. \tag{20}$$

Substituting (19) in (17), we obtain after transformations the following differential equation for $F(\mathbf{r}_\perp)$:

$$\Big(-\delta - \frac{\Delta_r}{2p(q-p)}\Big)F(\mathbf{r}_\perp) = (2\pi)^2\delta(\mathbf{r}_\perp) + \frac{1}{8\pi^4}\frac{1}{qv\varepsilon_0}\frac{e^2}{r_\perp}F(\mathbf{r}_\perp). \tag{21}$$

This is the equation for the Green's function of a two-particle with energy δ and mass $p(q-p)$, moving in a potential field $e^2/r_\perp$. Equation (21) is solved in the Appendix with the aid of the Laplace transformation. The answer is expressed in terms of the confluent hypergeometric function Ψ:

$$F(r_\perp)=4\pi p(q-p)e^{-r\beta}\Gamma(-\gamma)\Psi(-\gamma,1,2r_\perp\beta), \tag{22}$$

where

$$\beta^2=-\delta p(q-p),\quad \gamma=\alpha\sqrt{y(1-y)}-{}^1/_2,$$

$$y=\frac{p}{q}\qquad \alpha=\frac{1}{\sqrt{\delta}}\frac{\sqrt{2}}{16\pi^4}\frac{e^2}{v\varepsilon_0}.$$

At $r_\perp\to 0$ we have

$$F(r_\perp)=-4\pi p(q-p)\left[\ln r+\ln\sqrt{\delta}+\varphi(-\gamma)+\text{const}\right],$$
$$\varphi(x)=\frac{d}{dx}\ln\Gamma(x). \tag{23}$$

The term $p(q-p)\ln r$ leads to a term $q^2\ln r$ in Π; this reduces to a renormalization of the dialectic constant ϵ and is insignificant near the threshold.

The singular part of Π is equal to

$$\Pi_s=\frac{q^2}{v}\frac{1}{2\pi^2}K\left(\sqrt{\frac{qv}{qv-\omega}}\frac{\sqrt{2}}{8\pi^4}\frac{e^2}{v\varepsilon_0}\right), \tag{24}$$

where the universal function $K(\alpha)$ is given by

$$K(\alpha)=-\int_0^1 y(1-y)\left[-\ln\alpha+\varphi\left(\frac{1}{2}-\alpha\sqrt{y(1-y)}\right)\right]dy \tag{25}$$
$$=\frac{1}{6}\ln\alpha+\sum_{n=0}^{\infty}\left\{\frac{1}{2\alpha}\left[-c-\frac{\pi}{4}-\frac{\pi}{2}c^2+\frac{c^3}{\sqrt{c^2-1}}\left(\frac{\pi}{2}+\arcsin\frac{1}{c}\right)\right]-\frac{1}{6}\frac{1}{n+1}\right\},$$
$$c=(2n+1)/\alpha.$$

The imaginary part of $K(\alpha)$ for real α (i.e., at $\omega < qv$) has the simple form

$$\operatorname{Im}K(\alpha)=\frac{\pi}{4\alpha^3}\sum_{n=0}^{\left[\frac{\alpha-1}{2}\right]}\frac{(2n+1)^3}{\sqrt{\alpha^2-(2n+1)^2}}. \tag{26}$$

A plot of $\operatorname{Im}K(\alpha)$ is shown in Fig. 3.

Notice should be taken of an interesting phenomenon, namely infinite peaks at

$$qv-\omega=\frac{1}{(2n+1)^2}\times qv\left[\frac{\sqrt{2}}{16\pi^4}\frac{e^2}{v\varepsilon_0}\right]^2. \tag{27}$$

At these energy values, the electrons and holes form bound states in which the motion in a plane perpendicular to the total momentum is quantized, and the motion in the direction along the momentum is continuous, in analogy with the Landau levels.

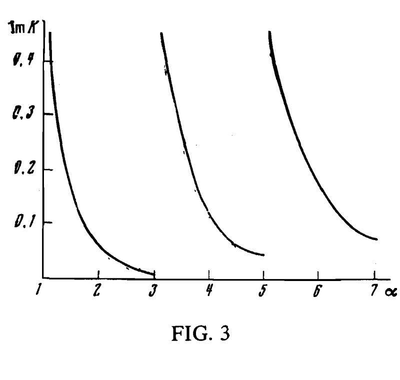


FIG. 3

In conclusion, we thank S. D. Beneslavskiĭ for valuable discussions and A. A. Migdal for directing the work.

APPENDIX

We rewrite (21) in the form

$$\left[-\delta-\frac{\Delta_r}{2p(q-p)}-\frac{\xi}{r_\perp}\right]F(\mathbf{r}_\perp)=\delta(\mathbf{r}_\perp)(2\pi)^2, \tag{A.1}$$

where

$$\xi=\frac{1}{8\pi^4}\frac{1}{qv}\frac{e^2}{\varepsilon_0},\quad \Delta_r=\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right).$$

Since $\delta(\mathbf{r}_\perp)=\delta(|\mathbf{r}_\perp|)/|\mathbf{r}_\perp|$, we can rewrite (A.1) in the form

$$\left\{\frac{-1}{2p(q-p)}\frac{d}{dr}\left(r\frac{d}{dr}\right)-(\delta r+\xi)\right\}F(r_\perp)=2\pi\delta(|\mathbf{r}_\perp|). \tag{A.2}$$

We apply to (A.2) the Laplace transformation

$$f(s)=\int_0 e^{-st}F(t)\,dt. \tag{A.3}$$

We obtain

$$\left[k\left(\frac{d}{dk}k\right)-\left(\beta^2\frac{d}{dk}+\xi_1\right)\right]f_1=1, \tag{A.4}$$

where

$$\beta^2=-2p(q-p)\delta,\quad \xi_1=2p(q-p)\xi,\quad f=4\pi p(q-p)f_1.$$

We seek the solution in the form

$$f_1=A\psi, \tag{A.5}$$

where ψ is a solution of the homogeneous equation

$$\psi=\left(\frac{k-\beta}{k+\beta}\right)^{\gamma}\frac{1}{k+\beta},\quad \gamma=\frac{1}{2}\left(\frac{\xi_1}{\beta}-1\right). \tag{A.6}$$

Substituting (A.6) in (A.5) and in (A.4), we obtain

$$f_1=\left(\frac{k-\beta}{k+\beta}\right)^{\gamma}\frac{1}{k-\beta}\int_0^k\frac{dp}{p-\beta}\left(\frac{p+\beta}{p-\beta}\right)^{\gamma}. \tag{A.7}$$

After the substitution

$$(p+\beta)/(p-\beta)=t(k-\beta)/(k+\beta) \tag{A.8}$$

we get

$$f_1=\int_0^1\frac{t^{-\gamma-1}}{k(1-t)+\beta(1+t)}dt. \tag{A.9}$$

To find $F(r_\perp)$, we must take the inverse Laplace transform

$$F(r_\perp)=4\pi p(q-p)\frac{1}{2\pi i}\int_{\eta-i\infty}^{\eta+i\infty}e^{kr_\perp}dk\int_0^1\frac{t^{-\gamma-1}dt}{k(1-t)+\beta(1+t)}. \tag{A.10}$$

Integrating in (A.10) with respect to k, we obtain

$$F(r_\perp)=4\pi p(q-p)\int_0^1\frac{t^{-\gamma-1}}{1-t}e^{-r\beta(1+t)/(1-t)}dt. \tag{A.11}$$

By means of the substitution $(1+t)/(1-t)=1+2y$ we reduce (A.11) to the more standard form

$$F(r_\perp)=4\pi p(q-p)e^{-r\beta}\int_0^1 y^{-\gamma-1}(1+y)^{\gamma}e^{-2\beta ry}dy \tag{A.12}$$
$$=4\pi p(q-p)e^{-r\beta}\Gamma(-\gamma)\Psi(-\gamma,1,2r\beta),$$

where Ψ is a confluent hypergeometric function.

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[1] A. A. Abrikosov and S. D. Beneslavskii, Zh. Eksp. Teor. Fiz. 59, 1280 (1970) [Sov. Phys.-JETP 32, 699 (1971)].

Translated by J. G. Adashko
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