Influence of magnetic field on excitonic transition

S. A. Gordyunin

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences
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It is shown within the framework of the Keldysh-Kopaev model with anisotropic band dispersion that the magnetic field hinders dielectric pairing. At low temperature, the transition to the dielectric field in a magnetic field is a first-order transition.

1. Different models of the metal–dielectric transition have been discussed many times in recent years. In particular, a transition to the dielectric phase takes place in a large number of oxides of transition metals and is accompanied by structural changes of the lattice. One of the models of the transition due to the singularities of the electron spectrum was proposed by Keldysh and Kopaev and by Kozlov and Maksimov [2], where the basic premise is the assumption of pairing of the electrons and holes having Fermi surfaces of the same shape, assumed in [1,2] to be spherical. However, the isotropy of the spectrum as such is immaterial here, and all that matters is the fact that the Fermi surfaces are congruent. This circumstance was independently used to understand a number of nontrivial properties of antiferromagnetism in chromium [3], for which purpose a model essentially in agreement with the premises of [1,2] was considered.

Gor'kov and Mnatsakanov [4] have previously [4] advanced the suggestion that the Keldysh–Kopaev model [1] is capable in principle of describing the appearance of small carrier groups. These considerations were based on the already known results [5,6] that any violation of the congruence of the Fermi surfaces weakens the tendency to dielectric pairing. It was therefore noted [5,7] that the dielectric transition of the type considered in [1] cannot be realized in the strongly anisotropic bismuth. It was asked instead whether the model of two coinciding Fermi surfaces can give rise to singularities of the electron spectra of V-group metals and semiconductors of the SnTe type.

A similar assumption concerning the electronic spectrum of bismuth was first advanced by Abrikosov and Fal'kovskiĭ [8] who carried out, in particular, a phenomenological analysis of the spectrum in the vicinities of high-symmetry points. Without stopping to compare the results of [7,8], we note that the most artificial factor in the model of [8] is the assumption that two electronic terms of generally speaking different symmetry coincide on the entire surface. For chromium, the presence of flat sections on the Fermi surface is usually attributed to the applicability of strongly-bound electrons to the model (see also [9]). In the case of bismuth [7] it was shown that the initial assumption that the electron and hole terms coincide in first order is a natural consequence of allowance for the singularities of the Coulomb interaction in the band theory.

We consider below, using the model of [1,2], the role of a sufficiently strong magnetic field. From the usual point of view, the action of a magnetic field on carriers in superconductors and semimetals consists of quantizing the motion of the quasiparticles. Therefore a field is strong if $\omega_c^* \sim \Delta$ or T, where Δ is the gap in the spectrum or the magnitude of the overlap, and $\omega_c^* = eH(c\partial S/\partial\epsilon)^{-1}$ [1]. It will be shown below that the considered model contains a somewhat unexpected parameter $\Lambda \sim (\omega_c^2 \epsilon_F)^{1/3}/T$ ($\omega_c = eH/mc$), which controls the values of the gaps and the volume of the Fermi surfaces. Therefore the dielectric undergoes in this model a transition to the metallic state prior to the onset of real quantization in sufficiently strong magnetic fields.

2. Just as in [4,7], we measure the spectrum of the electrons (zone 1) and of the holes (zone 2) along the normal to the Fermi surface

$$\xi_1(\mathbf{p}) = v_1(\mathbf{p}_F)\,t(\mathbf{p}_F) = v_1 t, \qquad \xi_2(\mathbf{p}) = -v_2(\mathbf{p}_F)\,t(\mathbf{p}_F) = -v_2 t, \tag{1}$$

where $t(\mathbf{p}_F)$ is the projection of the momentum on the positive direction of the normal to the Fermi surface, reckoned from the Fermi surface. The transition temperature T_{c0} in the absence of a field is determined by the condition that there exist a nonzero solution of the equation

$$\Delta(\mathbf{p}_F) = -T\sum_n \oint g(\mathbf{p}_F, \mathbf{p}_F')\,\Delta(\mathbf{p}_F')\,d\sigma' \int dt\, G_1 G_2 = \ln\frac{E_F}{T}\oint g(\mathbf{p}_F, \mathbf{p}_F')\,\Delta(\mathbf{p}_F')\frac{d\sigma'}{v_1(\mathbf{p}_F') + v_2(\mathbf{p}_F')}, \tag{2}$$

where E_F is the cutoff energy $\sim\epsilon_F$, and is immaterial in what follows.

In a magnetic field, the G-functions and Δ acquire an additional dependence on the coordinates. Let us consider the expression

$$\Pi(\mathbf{r}, \mathbf{r}') = -T\sum_n G_{1,i\omega_n}(\mathbf{r}, \mathbf{r}_1)\,\Delta(\mathbf{r}_1, \mathbf{r}_2)\,G_{2,i\omega_n}(\mathbf{r}_2, \mathbf{r}')\,d\mathbf{r}_1^3\,d\mathbf{r}_2^3. \tag{3}$$

Choosing $\mathbf{A} = -(1/2)\mathbf{r}\times\mathbf{H}$, we write down the equation for the G-function of the quasiparticles in the vicinity of the Fermi surface

$$\left\{i\omega_n - \xi\left(-i\frac{\partial}{\partial\mathbf{r}} + \frac{1}{2}\left[\mathbf{r}\frac{e\mathbf{H}}{c}\right]\right)\right\} G_{i\omega_n}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{4}$$*

After making the substitution

$$G_{i\omega_n}(\mathbf{r}, \mathbf{r}') = \exp\left(\frac{i}{2}\mathbf{r}'\left[\mathbf{r}\frac{e\mathbf{H}}{c}\right]\right)\tilde{G}_{i\omega_n}(\mathbf{r}, \mathbf{r}') \tag{5}$$

we see that $\tilde{G}_{i\omega n}(\mathbf{r}, \mathbf{r}')$ depends only on the coordinate difference $(\mathbf{r}-\mathbf{r}')$, so that we can go over to the momentum representation

$$\left\{i\omega_n - \xi\left(\mathbf{p} - \frac{i}{2}\left[\frac{d}{d\mathbf{p}}\frac{e\mathbf{H}}{c}\right]\right)\right\}\tilde{G}(\mathbf{p}, i\omega_n) = 1. \tag{6}$$

Expanding $\xi(\mathbf{p})$ near the Fermi surface up to terms of second order in H, corresponding to the usual weak-field assumption $\omega_c \ll T$, we obtain

$$\left\{i\omega_n - \xi + \lambda^3(\mathbf{p}_F)\frac{d^2}{d\xi^2}\right\}\tilde{G}(i\omega_n - \xi; \mathbf{p}_F) = 1, \tag{7}$$

$$\lambda^3(\mathbf{p}_F) = \frac{1}{2m_{ik}(\mathbf{p}_F)}\left[\mathbf{v}(\mathbf{p}_F)\frac{e\mathbf{H}}{c}\right]_i\left[\mathbf{v}(\mathbf{p}_F)\frac{e\mathbf{H}}{c}\right]_k. \tag{8}$$

In the derivation of (7) and (8) we used the fact that the term of first order in H is

$$\mathbf{v}(\mathbf{p}_F)\left[\frac{d}{d\mathbf{p}}-\frac{e\mathbf{H}}{c}\right]>0,$$

since $d\xi/d\mathbf{p}=\mathbf{v}(\mathbf{p}_F)$.

Using the fact that

$$\frac{d^2}{d\xi^2}G(i\omega_n\pm\xi)=\frac{d^2}{d(i\omega_n)^2}G(i\omega_n\pm\xi),$$

we write down final expressions for $\tilde{G}_1$ and $\tilde{G}_2$:

$$\begin{aligned}&\left\{i\omega_n-v_1t+\lambda_1{}^3\frac{d^2}{d(i\omega_n)^2}\right\}\tilde{G}_1(i\omega_n-v_1t;\ \mathbf{p}_F)=1,\\&\left\{i\omega_n+v_2t-\lambda_2{}^3\frac{d^2}{d(i\omega_n)^2}\right\}\tilde{G}_2(i\omega_n+v_2t;\ \mathbf{p}_F)=1.\end{aligned}\tag{9}$$

We turn to the definition of $\Pi(\mathbf{r},\mathbf{r}')$. Separating from all quantities in (3) the phase factor $\exp\{(1/2)i\mathbf{r}'\cdot\mathbf{r}\times\mathbf{H}\}$, we can easily verify that it is possible to go over to the momentum representation in $\tilde{\Pi}$ with sufficient accuracy. Indeed, after simple transformations we obtain

$$\begin{aligned}\tilde{\Pi}_{i\omega_n}(\mathbf{p})=&\int\tilde{G}_{1i\omega_n}(\mathbf{p}+\mathbf{k})\tilde{\Delta}(\mathbf{p})\tilde{G}_{2i\omega_n}(\mathbf{p}+\mathbf{q})\delta(k_z)\\&\times\delta(q_z)\frac{1}{H^2}\exp\left(\frac{i}{H^2}[\mathbf{kq}]\mathbf{H}\right)d^3k\,d^3q.\end{aligned}\tag{10}$$

The z axis determines here the direction of $\mathbf{H}$.

Since $\tilde{G}_1(\mathbf{p}+\mathbf{k})$ and $\tilde{G}_2(\mathbf{p}+\mathbf{q})$ depend on $\mathbf{k}$ and $\mathbf{q}$ via $\mathbf{v}_1\cdot\mathbf{k}$ and $\mathbf{v}_2\cdot\mathbf{q}$, it follows that by choosing $\mathbf{v}_1(\|\mathbf{v}_2)$ to lie, for example, in the xz plane, we find after integrating with respect to k_y and q_y that

$$\tilde{\Pi}(\mathbf{p})=\tilde{G}_1(\mathbf{p})\tilde{\Delta}(\mathbf{p})\tilde{G}_2(\mathbf{p}).$$

To determine T_c in the field H we have in place of (2) the equation

$$\tilde{\Delta}(\mathbf{p}_F)=-T\sum_n\oint g(\mathbf{p}_F,\mathbf{p}_F')\tilde{\Delta}(\mathbf{p}_F')\int dt\,\tilde{G}_1(i\omega_n-v_1t)\tilde{G}_2(i\omega_n+v_2t).\tag{11}$$

Let us consider the expression

$$\Phi(\omega_n)=\int dt\,\tilde{G}_1\tilde{G}_2.$$

We multiply the first equation of (9) by $v_2\tilde{G}_2$, and the second by $v_1\tilde{G}_1$, add the two and integrate with respect to t. It is easy to verify that $\int G_1dt$ and $\int G_2dt$ are equal to their value in the absence of a field. (The density of the number of states does not change). We note furthermore that

$$\frac{d^2\tilde{G}_\alpha}{d(i\omega_n)^2}=\frac{1}{v_\alpha{}^2}\frac{d^2G_\alpha}{dt^2},\quad\alpha=1,2,$$

After certain transformations we obtain the equation

$$\begin{aligned}&i\lambda^3\frac{d^2}{d\omega_n{}^2}\Phi'+\omega_n\Phi'=-\operatorname{sign}\omega_n,\\&\Phi'(\omega_n)=\frac{v_1+v_2}{2\pi}\Phi(\omega_n),\end{aligned}\tag{12}$$

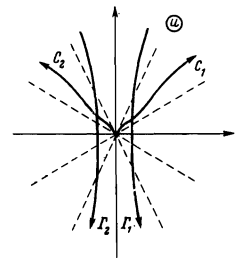
$$\lambda^3(\mathbf{p}_F)=\frac{1}{2}\left[\mathbf{v}\frac{e\mathbf{H}}{c}\right]_i\left[\mathbf{v}\frac{e\mathbf{H}}{c}\right]_k\left(\frac{v_2}{m^{(1)}_{ik}}-\frac{v_1}{m^{(2)}_{ik}}\right),\quad\mathbf{v}=\frac{\mathbf{v}_1v_2}{v_1+v_2}.\tag{13}$$

In the case of a quadratic dispersion law in both bands we have $\lambda^3(\mathbf{p}_F)=0$. (For spheres we have $m_2v_2=m_1v_1=p_0$).

Using the Laplace method, we write down directly the solutions for $\Phi'(\omega_n>0)$ and $\Phi'(\omega_n<0)$:

$$\begin{aligned}\Phi'(\omega_n>0)=&\int_{C_1}\exp\left[\omega_nu+\frac{i(\lambda u)^3}{3}\right]du,\\\Phi'(\omega_n<0)=&\int_{C_2}\exp\left[\omega_nu+\frac{i(\lambda u)^3}{3}\right]du.\end{aligned}\tag{14}$$

The contours C_1 and C_2 are chosen such as to obtain



the correct asymptotic form in ω_n (see the figure). Summing over the frequency and separating $\Phi_0'=-1/|\omega_n|$, we obtain

$$\begin{aligned}\Phi'(\mathbf{p}_F)=T\sum_n\Phi'(\omega_n)=&\ln\frac{E_F}{T}-\frac{1}{2}\int_0^\infty\frac{du}{\operatorname{sh}\pi u}\left(1-\cos\frac{(\Lambda u)^3}{3}\right),\\\Lambda(\mathbf{p}_F)=&\frac{\lambda(\mathbf{p}_F)}{T}\approx\frac{(\omega_c{}^2\varepsilon_F)^{1/3}}{T}.\end{aligned}\tag{15}$$

When $\Lambda\ll1$ (weak fields) we get

$$\Phi'(\mathbf{p}_F)=\ln\frac{E_F}{T}-\frac{635\zeta(7)}{16\pi^7}\Lambda^6(\mathbf{p}_F)\tag{16}$$

and thus

$$T_c=T_{c0}\left(1-\frac{635\zeta(7)}{16\pi^7}\overline{\Lambda^6}\right)$$

where the bar denotes averaging as in [4]:

$$\begin{aligned}\overline{(\ldots)}=&\oint\frac{d\sigma}{v_1+v_2}|\chi(\mathbf{p}_F)|(\ldots),\\&\oint|\chi(\mathbf{p}_F)|^2\frac{d\sigma}{v_1+v_2}=1.\end{aligned}$$

If $\Lambda\gg1$ but $\omega_c\ll T$, we can obtain for Φ' the asymptotic expression

$$\begin{aligned}&\Phi'(\mathbf{p}_F)=\ln\frac{E_F}{T}-\ln\frac{\lambda}{T}+c\left(\frac{T}{\lambda}\right)^2,\quad c=\frac{\Gamma(^2/_3)\pi^2\,3^{1/3}}{48}\\&T_c(H)=(\lambda_c/c)^{1/3}(\lambda-\lambda_c)^{1/3},\quad\lambda_c=T_{c0},\end{aligned}\tag{17}$$

i.e., a nonzero solution for the gap exists at fields stronger than H_c.

3. The dependence of all the properties on the magnetic field and, in particular, the spectrum, can be obtained if we know the solutions of the system of equations for the Green's functions

$$\begin{aligned}\tilde{G}_{11}(\mathbf{p})=&\tilde{G}_1(\mathbf{p})+\tilde{G}_1(\mathbf{p})\tilde{\Delta}(\mathbf{p})\tilde{G}_{21}(\mathbf{p}),\\\tilde{G}_{21}(\mathbf{p})=&\tilde{G}_2(\mathbf{p})\tilde{\Delta}^*(\mathbf{p})\tilde{G}_{11}(\mathbf{p}).\end{aligned}$$

The formal solution is

$$\tilde{G}_{11}(\mathbf{p})=\frac{\tilde{G}_1(\mathbf{p})}{1-|\Delta|^2\tilde{G}_1(\mathbf{p})\tilde{G}_2(\mathbf{p})},\quad G_{21}(\mathbf{p})=\frac{\Delta^*(\mathbf{p})}{1-|\Delta|^2\tilde{G}_1(\mathbf{p})\tilde{G}_2(\mathbf{p})}.\tag{18}$$

The actual investigation of the singularities of expressions (18) on the real axis, however, is a complicated problem. Even to find $G^{R(A)}_{1,2}$ it is necessary to solve (9) with the substitution $i\omega_n\to\epsilon$, so as to make the solution analytic in the upper (lower) ϵ half-plane, and furthermore, for the solution to decrease asymptotically with $(\epsilon\pm v_2t)$. Expressions (18) are made complicated by the possible existence of poles. To understand qualitatively the character of the variation of the dielectric-phase spectrum with changing field, let us consider, in the case of weak fields, the spectrum near the excitation threshold:

$$\varepsilon_0=\Delta\frac{2\sqrt{v_1v_2}}{v_1+v_2},\quad t_0=\frac{\Delta|v_1-v_2|}{(v_1+v_2)\sqrt{v_1v_2}}.\tag{19}$$

In this case we have

$$\bar{G}_\alpha^{R}=(\varepsilon\pm v_\alpha t)^{-1}+\operatorname{Im}\bar{G}_\alpha^{R},\quad \alpha=1,\ 2.$$

For $\tilde{G}_1^R$ and $\tilde{G}_2^R$ we have

$$\operatorname{Im}\bar{G}_1^{R}=\frac{1}{2}(\bar{G}_1^{R}-\bar{G}_1^{A})=\theta(v_1 t-\varepsilon)\int_{\Gamma_1}\exp\left[(\varepsilon-v_1 t)u+\frac{(\lambda_1 u)^3}{3}\right]du,$$

$$\operatorname{Im}\bar{G}_2^{R}=\frac{1}{2}(\bar{G}_2^{R}-\bar{G}_2^{A})=\theta(v_2 t+\varepsilon)\int_{\Gamma_2}\exp\left[(\varepsilon+v_2 t)u-\frac{(\lambda_2 u)^3}{3}\right]du.$$

For the spectrum near the threshold we obtain a finite imaginary part

$$\varepsilon=\varepsilon_0\left\{1+i\alpha\left(\frac{\Delta}{\lambda_1}\right)^{3/4}\exp\left[-\left(\frac{\Delta}{\lambda_1}\right)^{3/2}\right]+i\beta\left(\frac{\Delta}{\lambda_2}\right)^{3/4}\exp\left[-\left(\frac{\Delta}{\lambda_2}\right)^{3/2}\right]\right\},\quad \alpha,\beta\approx 1. \tag{20}$$

This result evidently denotes a gapless character of the system spectrum. The density of states at $\epsilon=0$ is also finite, albeit exponentially small:

$$\rho(0)\sim\rho_0(0)\left(\frac{\Delta}{\lambda}\right)^{3/4}e^{-(\Delta/\lambda)^{3/2}}.$$

It is impossible to trace the behavior of the density of states over the entire field interval, all the more since, according to (16), at $\bar{\lambda}\sim\bar{\lambda}_c=T_{c0}$ in our picture the transition from the dielectric phase to the semimetallic state at low temperatures turn out to be a first-order transition. Attention should be called, however, to the fact that in the vicinity of large fields and low temperatures it appears that a superstructure can be formed with a period $q^*\sim T_c/v_F$, analogous to the superstructure in the superconductor in the exchange field [12].

In concluding this section we note once more that the considered effect is connected directly with the anisotropy of the system and is absent in the case of a quadratic spectrum. In the latter case, as is well known, it would be possible to changeover to the mass-center coordinates, and the pairing of the electron with the hole would not be very sensitive to the magnetic field because the magnetic field does not act on a neutral formation. In the case when there is an anisotropy of general form, the coordinates of the mass center, as such, do not exist. It seems to us that this effect can be regarded as quantum motion of an electron-hole pair and in this sense it resembles, for example, the influence of a strong magnetic field on the critical temperature in a superconductor.

4. As a result of the exciton transition, a semimetal may be produced with Fermi surfaces in the form of lobes [7] (one dimension $\sim T_c/v_F$ and two others large $\sim p_0$). We compare, for such a semimetal, the role of the quantum effects and of the obtained band-motion effect. The magnitude of the quantum effects is determined by the parameter ω_c^*/T, where $\omega^*=eH/m^*c$. For the indicated form of the spectrum we have $m^*\sim m$ and the quantum effects do not have time to develop in such a semimetal. The spectrum on Bi is more complicated. Therefore the quantization in the field turns out to be appreciable at $\Lambda\sim 1$. However, the relative change of the band positions might be controlled by the described effect. In addition, apart from the pure methodological interest that might attach to the result, it can be assumed that the Fermi surfaces in Sb and As have shapes close to those given by this model.

In conclusion, I am grateful to L. P. Gor'kov for help with the work.

*$\left[\mathbf{r}\frac{e\mathbf{H}}{c}\right]\equiv\mathbf{r}\times(e\mathbf{H}/c)$.

[1)]The dielectric pairing in quantizing fields ($\omega_c\gg T$) was investigated by Abrikosov [10] and by Brazovskiĭ [11].

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