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CONTRIBUTION TO THE THEORY OF BAND FERROMAGNETISM

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Submitted 10 December 1973
ZhETF Pis. Red. 19, No. 3, 168 — 171 (5 February 1974)

A model is investigated with a single-electron spectrum that is unstable against electron-hole pairing. Conditions are found under which the singlet and triplet electron-hole pairing can coexist and lead to a ferromagnetic state of collectivized conduction electrons.

It is known that in the approximation of a simple parabolic electron band $\varepsilon(\vec{p}) = p^2/2m$ the ferromagnetic state resulting from Coulomb interaction between conduction electrons is possible only if the interaction is strong enough [1, 2].

The magnetization of the electron gas, say in the x direction, can be expressed in the form

$$M_x \sim -i \sum_\sigma \int \frac{d^3q}{(2\pi)^3} G_{-\sigma,\sigma}(q, -0), \qquad (1)$$

where

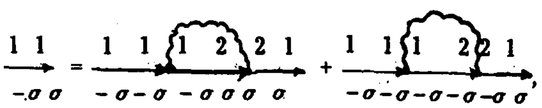
$$G_{-\sigma,\sigma} = -i < Ta_{-\sigma}(t)a^+_\sigma(0) > .$$

We shall discuss below substances having a one-electron spectrum with singular properties, namely either semimetals with almost coinciding electron and hole Fermi surfaces [3], or semiconductors with a forbidden band much smaller than the exciton binding energy [4], or else metals with narrow allowed bands, when the condition $\varepsilon(\vec{p}) = -\varepsilon(\vec{p} + \vec{q})$ is approximately satisfied [5].

We shall show that a transition to the ferromagnetic semiconducting state is possible for such systems even in the case of weak interaction. The ferromagnetism is brought about here by the collectivized electrons of the conduction band of the doped semiconductor.

In all the listed cases, at an arbitrarily weak interelectron in-eraction, the system is unstable against electron-hole pairing in either the singlet state, characterized by an anomalous Green's function $G^{21}_{\sigma\sigma} = -i<Ta_{2\sigma}a^+_{1\sigma}>$ and a binding potential V_C, or in a triplet state characterized by an anomalous function $G^{21}_{-\sigma\sigma} = -i<Ta_{2-\sigma}a^+_{1\sigma}>$ with a potential V_T (the subscripts 1 and 2 characterize here either the numbers of the bands [3, 4] or two states that differ by the vector $\vec{q}$).

It will be shown below that singlet and triplet electron-hole pairings can exist in the case of a doped semimetal [3] or semiconductor [4], or else in the case of a metal in which the number of electrons per unit cell differs slightly from unity. But in this case the functions $G^{11}_{-\sigma\sigma}$ and $G^{22}_{-\sigma\sigma}$, which characterize the magnetization in accordance with (1), also turn out to be different from zero at arbitrarily weak interaction, as can be easily seen from the following formal equation:



$$(G^{11}_{\sigma\sigma} = G^{11(0)}_{-\sigma-\sigma} V_T G^{12}_{-\sigma\sigma} G^{21}_{\sigma\sigma} + \dots). \tag{2}$$

From the system of equations for the Green's functions, analogous to Eq. (2), we can obtain the excitation spectrum:

$$\omega_{\pm}^2 = \epsilon^2(\mathbf{p}) + (\Delta_c + \Delta_T)^2 \tag{3}$$

of the system of equations for the singlet (Δ_C) and triplet (Δ_T) dielectric gaps

$$\ln\frac{\tilde{\omega}}{\Delta_T^0} = \frac{1}{2}\left(1 - \frac{\Delta_c}{\Delta_T} + \frac{\Delta_T}{\Delta_c}\right)\ln\frac{\tilde{\omega}}{\sqrt{\delta\mu^2 - (\Delta_c + \Delta_T)^2} + \delta\mu} + \frac{1}{2}\left(1 + \frac{\Delta_c}{\Delta_T} - \frac{\Delta_T}{\Delta_c}\right)\times$$

$$\times \ln\frac{\tilde{\omega}}{\sqrt{\delta\mu^2 - (\Delta_c - \Delta_T)^2} + \delta\mu}$$

$$\ln\frac{\tilde{\omega}}{\Delta_c^0} = \frac{1}{2}\left(1 + \frac{\Delta_c}{\Delta_T} - \frac{\Delta_T}{\Delta_c}\right)\ln\frac{\tilde{\omega}}{\sqrt{\delta\mu^2 - (\Delta_c + \Delta_T)^2} + \delta\mu} + \frac{1}{2}\left(1 - \frac{\Delta_c}{\Delta_T} + \frac{\Delta_T}{\Delta_c}\right)\times \tag{4}$$

$$\times \ln\frac{\tilde{\omega}}{\sqrt{\delta\mu^2 - (\Delta_c - \Delta_T)^2} + \delta\mu},$$

and the electroneutrality condition

$$[\delta\mu^2 - (\Delta_T + \Delta_c)^2]^{1/2} + [\delta\mu^2 - (\Delta_T - \Delta_c)^2]^{1/2} = n . \tag{5}$$

Here n is the concentration of the doping impurity, $\delta\mu$ characterizes the shift of the Fermi level relative to the center of the forbidden band as a result of the doping. The branches ω_+ and ω_0 characterize states with spins up and down, respectively, i.e., spin splitting and the associated magnetization take place.

We consider first the case of an undoped semimetal (semiconductor). We find on the phase diagram (Δ_c^0, Δ_T^0) (Fig. 1) the line on which $\Delta_c = 0$. Here $\Delta_c^0(\Delta_T^0)$ is the value of the singlet (triplet) dielectric gap in the absence of a triplet (singlet) one. In this case we obtain from (4)

$$\ln|\Delta_c^0/\Delta_T^0| = 1, \quad \ln|\Delta_T^0/\Delta_T| = 0, \text{ i.e., } \Delta_T = \Delta_T^0 = e^{-1}\Delta_c^0 . \tag{6}$$

For the line $\Delta_T = 0$ we have analogously $\Delta_c = \Delta_c^0 = e^{-1}\Delta_T^0$ (Fig. 1).

Thus, the region of the coexistence of Δ_c and Δ_T lies between the lines with slopes e and e^{-1}. In the coexistence region, the growth, say of the value of Δ_c, as can be easily seen from Fig. 1, takes place when the potential V_c decreases, i.e., when Δ_c^0 decreases, which is unphysical. Actually, an analysis of the free energy, similar to the analysis in the case of the coexistence of dielectric and superconducting pairings in an undoped semimetal [7] shows that the region of coexistence cannot be realized even as a metastable state.

The corresponding analysis for the line $\Delta_c = 0$ in the case of a doped semimetal leads to the following equations in place of (6):

$$\ln|\Delta_c^0/\Delta_T^0| = 2\Delta_T^2 n^{-1}\left(\sqrt{\Delta_T^2 + n^2} + n\right)^{-1},$$

$$(\Delta_T^0\,\Delta_c^0)^{1/2} = \sqrt{\Delta_T^2 + n^2} + n, \tag{7}$$

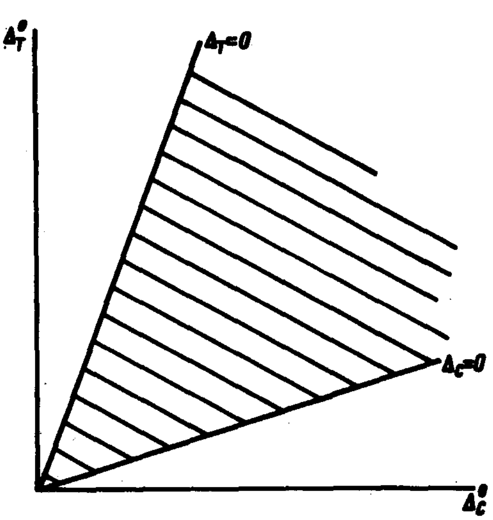


Fig. 1

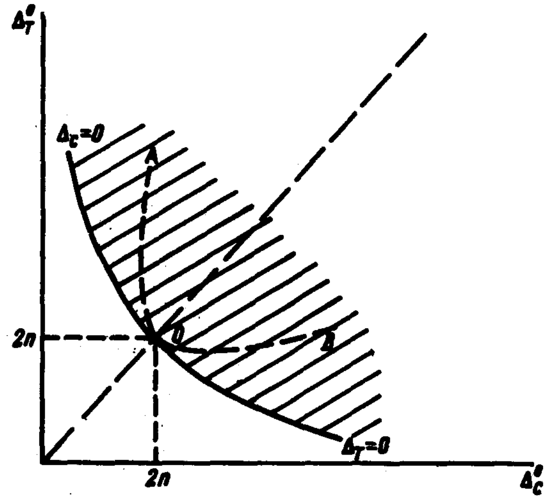


Fig. 2

i.e., $\Delta_T = (\Delta_T^0\Delta_C^0 - 2n\sqrt{\Delta_T^0\Delta_C^0})^{1/2}$, and $\Delta_C = 0$ on the line (Fig. 2):

$$\ln|\Delta_C^0/\Delta_T^0| = -2n^{-1}(\sqrt{\Delta_T^0\Delta_C^0} - 2n). \tag{8}$$

Expressions similar to (7) and (8), with the substitution $\Delta_C^0 \rightleftarrows \Delta_T^0$, are obtained for the line $\Delta_T = 0$ (the section of the curve on Fig. 2 below the bisector; the coexistence region is shaded).

Thus, a growth of the quantity Δ_C, for example, takes place when the potential V_C (or Δ_C^0) increases. An analysis of the expression for the free energy near the bisector ($\Delta_C^0 \approx \Delta_T^0$) shows that the ferromagnetic state is energywise favored in comparison with the case of a separate solution for $\Delta_C \neq 0$ or $\Delta_T \neq 0$. The line AOB, the determination of which calls for numerical calculations, is a line of first-order transition from the ferromagnetic to the paramagnetic state. On the other hand, the lines $\Delta_C = 0$ and $\Delta_T = 0$ are "superheat" lines and in the region between them and the line AOB the ferromagnetic state of the system is metastable.

The magnetization of the system and the Curie temperature are proportional to the degree of doping n (at $n/\Delta^0 \ll 1$). To describe the possible ferromagnetic behavior of the compounds of the A_4B_6 group, it is necessary to take the hybridization effects into account [8].

The considered model explains qualitatively the magnetic properties of semiconductors with narrow forbidden bands when the semiconductors are doped [9], and is an alternative to the theory of [10].

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