significant at low temperatures $T \ll \Theta$ and frequencies $\omega \ll \omega_D$. However, for sufficiently low frequencies, Eq. (5) for the electrical conductivity is invalid as the result of the anomalous skin effect. It was shown in the work of Motulevich[8] that the corrections to the surface impedance associated with the anomaly are small if the quantity $\frac{3}{8}(v_F/c)[1 + (n/\chi)^2]^{1/2}[1 + (\nu/\omega)^2]^{-1/2}$ (n and χ are the real and imaginary parts of the index of refraction) is smaller than or of the order of unity. For $\omega \gg \nu$, this condition leads to the following limitation on the frequency of the electromagnetic field: $\omega \gtrsim 10^{13}$ Hz.

Up to now we have considered the case of comparatively high frequencies of the electromagnetic field, for which $\omega\tau \gg 1$. We shall show that the dependences of the frequency of the electron-phonon collisions on the temperature, obtained above, are also valid for the static electrical conductivity if collisions of electrons with impurities are predominant. In this case, the small contribution to the distribution function of the electrons, which is associated with electron-phonon collisions, can be determined by iteration of the kinetic equation.

If we assume that each collision of an electron with an impurity is "effective" (i.e., the mean momentum transferred to the electron in the collision is of the order of p_F), then we get for the resistivity $\rho = 1/\sigma$,

$$\rho = m(\nu_{ei} + \nu_{ep}) / e^2N.$$

In this formula, ν_{ei} is the frequency of collisions of electrons with impurities, and the frequency of the electron-phonon collisions $\nu_{ep}(T) = \nu_0 + \nu_I + \nu_{II}$, where the quantities ν_0, ν_I and ν_{II} are determined by Eqs. (6), (8), and (10) in their temperature dependence and their order of magnitude; here one must set $\omega = 0$ (exact agreement is obtained if the approximation of the relaxation time is applicable for collisions of electrons with impurities).

The author expresses his deep gratitude to R. N. Gurzhi for direction of the given work.

---

[1] R. N. Gurzhi, Zh. Eksp. Teor. Fiz. **33**, 660 (1957) [Sov. Phys.-JETP **6**, 506 (1958)].

[2] E. Pytte, J. Phys. Chem. Sol. **28**, 93 (1967).

[3] V. F. Gantmakher and Yu. S. Leonov, ZhETF Pis. Red. **8**, 264 (1968) [JETP Lett. **8**, 162 (1968)].

[4] A. N. Friedman, Phys. Rev. **159**, 553 (1967).

[5] W. Harrison, The Pseudopotential in the Theory of Metals, Benjamin, 1966.

[6] L. J. Sham and J. M. Ziman, Sol. State Phys. **15**, 221 (1963).

[7] R. N. Gurzhi, Zh. Eksp. Teor. Fiz. **33**, 451 (1957) [Sov. Phys.-JETP **6**, 352 (1958)].

[8] G. P. Motulevich, Zh. Eksp. Teor. Fiz. **46**, 273 (1964) [Sov. Phys.-JETP **19**, 189 (1964)].

Translated by R. T. Beyer
147

SOVIET PHYSICS JETP VOLUME 32, NUMBER 4 APRIL, 1971

POSSIBLE EXISTENCE OF SUBSTANCES INTERMEDIATE BETWEEN METALS AND DIELECTRICS

A. A. ABRIKOSOV and S. D. BENESLAVSKIĬ

L. D. Landau Institute of Theoretical Physics

Submitted April 13, 1970

Zh. Eksp. Teor. Fiz. 59, 1280–1298 (October, 1970)

The question of the possible existence of substances having an electron spectrum without any energy gap and, at the same time, not possessing a Fermi surface is investigated. First of all the question of the possibility of contact of the conduction band and the valence band at a single point is investigated within the framework of the one-electron problem. It is shown that the symmetry conditions for the crystal admit of such a possibility. A complete investigation is carried out for points in reciprocal lattice space with a little group which is equivalent to a point group, and an example of a more complicated little group is considered. It is shown that in the neighborhood of the point of contact the spectrum may be linear as well as quadratic.

The role of the Coulomb interaction is considered for both types of spectra. In the case of a linear dispersion law a slowly varying (logarithmic) factor appears in the spectrum. In the case of a quadratic spectrum the effective interaction becomes strong for small momenta, and the concept of the one-particle spectrum turns out to be inapplicable. The behavior of the Green's functions is determined by similarity laws analogous to those obtained in field theory with strong coupling and in the neighborhood of a phase transition point of the second kind (scaling). Hence follow power laws for the electronic heat capacity and for the momentum distribution of the electrons.

1. INTRODUCTION

ONE of the basic assumptions of the Landau[1] theory of a Fermi liquid is the relationship, according to which the limiting momentum of the excitations in an isotropic Fermi liquid is determined in the same way as in a gas, by the density of the atoms in the liquid, i.e., $p_0 = (3\pi^2 n)^{1/3}$ (where n is the density of particles). According to the work of Luttinger and Ward,[2] with a certain amount of alteration this theorem is also applicable to the electronic liquid in metals. Namely, it turns out that the total volume, bounded by all Fermi surfaces, determines the density of the electrons:

$$n = 2(2\pi)^{-3}(pV_0 + V_F),$$

where V_0 denotes the volume of an elementary cell of the reciprocal lattice, p is an integer, and V_F denotes the total volume inside all of the Fermi surfaces (from the side of smaller energies), referred to a single cell of the reciprocal lattice.

It is not difficult to see that the cited relation is exactly the same as for a noninteracting Fermi system in a periodic field. In view of the fact that $V_0 = (2\pi)^3/v$, where v is the volume of an elementary cell of the crystal, the substance can be dielectric only when the number of electrons per elementary cell of the crystal is even. If in this case the substance nevertheless is a metal, then the number of holes must necessarily be equal to the number of electrons. For metals with an odd number of electrons per cell, on the other hand, such compensation cannot occur.

In this connection the question arises whether substances can exist in nature which are neither genuine metals nor dielectrics in the sense that there are no free electrons in them, and at the same time no energy gap is present. One can represent such a substance as the limiting case of a metal with a point Fermi surface. In the language of the theory of noninteracting particles in a periodic field, this corresponds to the case when a completely filled valence band touches a completely empty conduction band. Indications of the possible existence of such substances have recently appeared in the literature (gray tin[3] and mercury telluride[4]).

In the present article the conditions under which a point Fermi surface may appear in a model of noninteracting electrons will be investigated, and the question of the influence of the Coulomb interaction of the electrons on the energy spectrum in the neighborhood of the Fermi point will be considered.

In the case of interest to us, the maximum of the valence band must coincide with the minimum of the conduction band. In general an increased symmetry of the appropriate point of the reciprocal lattice favors degeneracy of the energy levels, but it may also occur at accidental points. However, here somewhat more is required, namely, that this point simultaneously corresponds to extrema of the two bands. The occurrence of such a situation at an accidental point is an improbable special case. In view of this we shall consider only "regular" cases, i.e., points of high symmetry. A complete analysis is given in the case when the little group of the corresponding point is equivalent to the point group, and an example of a more complicated group is considered. It turns out that a "Fermi point" is possible in a whole series of different cases, where in the most typical cases the dispersion law in the vicinity of such a point will either be linear or quadratic.

However, in general a model of noninteracting electrons does not correspond to a real electronic liquid. In the case of an isotropic liquid with short-range interaction forces, Landau was able to show (see[5]) that the energy spectrum of the quasi-particles retains the same form as for a Fermi gas. This proof was then generalized to a Fermi liquid in a crystal[2,6] and to a Fermi liquid with long-range Coulomb forces.[7] In the last case the fact that the presence of "free electrons" leads to a screening of the Coulomb field and converts it into a short-range field is extremely important. Close-lying excited states play the most important role in the integral which determines the screening. Therefore, in any case the screening is absent if there is a gap in the spectrum. On the other hand, in a real metal the screening radius is of the order of interatomic distances.

From this point of view it is necessary to investigate what kind of influence the Coulomb field has in the case of a "Fermi point." The absence of any gap in the spectrum must necessarily lead to a weakening of the Coulomb potential at large distances. At the same time the replacement of the Fermi surface by a point leads to a change in the nature of the screening, and it is not obvious beforehand how this will affect the energy spectrum.

The usual way to prove the presence of a Fermi spectrum in the theory of a Fermi liquid (see[5]) consists in the following. It is assumed that the spectrum has the appropriate form and, starting from this, the Green's function is written down. After this it is proved that the constant coefficients appearing in it are actually constants which depend on the interaction of the particles. This method of proof is universal for that case when one can foresee the result beforehand. However, in the case under consideration this is by no means so. Therefore, let us proceed according to a different method. Let us consider the Coulomb interaction, which we shall assume to be weak and, using the Green's function of noninteracting particles as the zero-order approximation, let us find the Green's function and the other characteristic quantities associated with the presence of the interaction.

The supposition about the weakness of the interaction may be justified by the following consideration. In the cases under consideration there exists a large range of momenta for which the valence band is close to the conduction band. As we shall see below, in the very neighborhood of the point of contact between the bands a nontrivial situation arises which, in particular, leads to a change in the nature of the interaction at small values of the momenta. However, the nearness of the bands is preserved even at a certain distance from this neighborhood. If we shall consider the electronic transitions outside the "dangerous neighborhood", then they lead to the appearance of the ordinary dielectric constant ϵ_0 which, in view of the proximity of the bands, should be rather large (as, for example, in Ge and Si). In view of this the bare Coulomb interaction $e^2/\epsilon_0 r$ or, more precisely, the characteristic dimensionless constant $e^2/\epsilon_0 v$, where $v \sim 10^8$ cm/sec, must be small. Of course, in addition the case is possible when the dielectric constant is not large and consequently the interaction will not be weak which, in turn, leads to an increase of the "dangerous neighborhood" up to dimensions which are comparable with the period of the reciprocal lattice. However, to judge from the existing data on α-Sn and HgTe, this case scarcely occurs. But even if ϵ_0 is not overly large then, in any case, with the aid of a study of the weakened interaction one can formulate some idea about what happens in the neighborhood of the Fermi point.

We have considered the two most typical cases: linear and quadratic spectra in the neighborhood of the contact point. It turns out that both types of spectra lead to quite different consequences upon taking the interaction into account. One can assume that these two characteristic types of behavior exhaust all possibilities.

2. CONTACT IN THE GROUPS D_n

First of all let us consider a point k_0 in reciprocal lattice space with a little group which is equivalent to one of the point groups. Since the question involves the contact of bands, then degeneracy of the levels must occur at the point k_0, which is lifted (if only partially) upon a change of k in an arbitrary direction. This means that the little group of k_0 must have a multidimensional representation, i.e., contain axes of the third, fourth, or sixth orders. In addition, it is obvious that an intersection of the axes and planes of symmetry must occur at the point k_0. If the spin-orbit coupling is small enough so that one can neglect it, then it is necessary to consider single-valued irreducible representations. Upon taking account of the spin-orbit coupling it is necessary to consider double-valued representations.

Let us start with simple groups. Let us demonstrate that contact is possible in the groups D_3, D_4, and D_6. As is shown in article[5], in order to determine the dispersion law it is necessary to construct an invariant form $Q(\mathbf{k}; \mathbf{r}, \mathbf{r}')$ containing the components of the vector k and which is bilinear in the basis functions $u_\alpha(\mathbf{r})$ and $u_\alpha^*(\mathbf{r}')$. Let us consider single-valued representations. In the groups under consideration, one invariant exists which is linear in k: $[u_+(\mathbf{r})u_+^*(\mathbf{r}') - u_-(\mathbf{r})u_-^*(\mathbf{r}')]k_z$. The presence of such an invariant is very important because it is precisely this property which guarantees the possibility of a "Fermi point", where the functions $u_\pm$ transform like $x \pm iy$. With the components k_x and k_y one can form only the quadratic invariants

$$u_+(\mathbf{r})u_-^*(\mathbf{r}')k_-^2 + u_-(\mathbf{r})u_+^*(\mathbf{r}')k_+^2, \quad k_\pm = k_x \pm ik_y$$

and

$$[u_+(\mathbf{r})u_+^*(\mathbf{r}') + u_-(\mathbf{r})u_-^*(\mathbf{r}')]k_\perp^2, \; k_\perp^2 = k_x^2 + k_y^2.$$

Since the latter combination of $u_\pm$ is an invariant by itself, then one can also multiply it by the invariant k_z^2. Finally the invariant

$$u_+(\mathbf{r})u_-^*(\mathbf{r}')k_+^2 + u_-(\mathbf{r})u_+^*(\mathbf{r}')k_-^2.$$

still exists in the group D_4. Collecting everything together one can write down the following invariant form:

$$\begin{aligned} Q(\mathbf{k};\, \mathbf{r},\, \mathbf{r}') = {} & [u_+(\mathbf{r})u_+^*(\mathbf{r}') + u_-(\mathbf{r})u_-^*(\mathbf{r}')](\alpha k_\perp^2 + \beta k_z^2) \\ & + \nu[u_+(\mathbf{r})u_+^*(\mathbf{r}') - u_-(\mathbf{r})u_-^*(\mathbf{r}')]k_z + \\ & + \gamma[u_+(\mathbf{r})u_-^*(\mathbf{r}')k_-^2 + u_-(\mathbf{r})u_+^*(\mathbf{r}')k_+^2] \\ & + \delta[u_+(\mathbf{r})u_-^*(\mathbf{r}')k_+^2 + u_-(\mathbf{r})u_+^*(\mathbf{r}')k_-^2]. \end{aligned} \tag{1}$$

In the groups D_3 and D_6 the coefficient $\delta = 0$. Putting together the secular equation, we obtain the following result for the energy levels:

$$\varepsilon_{1,2} = \alpha k_\perp^2 + \beta k_z^2 \pm [\nu^2 k_z^2 + (\gamma + \delta)^2 k_\perp^4 - 8\delta\gamma k_x^2 k_y^2]^{1/2}. \tag{2}$$

It is not difficult to see that ranges of values of the coefficients exist for which one of the branches is positive for all directions k and the other is negative, i.e., a point Fermi surface is possible. It is of interest to note that the behavior of the branches of the spectrum is strongly anisotropic. In a direction outside the basis plane $\epsilon_{1,2}$ changes basically according to a linear law, but in the basis plane it changes according to a quadratic law.

In the presence of strong spin-orbit coupling it is necessary to use double-valued representations. Two double-valued representations exist in the group D_3 (see[6]). With the aid of the basis functions for the representation E_2', which transform like the components of a spinor, one can set up invariants which are linear in k_z and $k_\pm$. The general invariant form has the form

$$\begin{aligned} Q(\mathbf{k};\, \mathbf{r},\, \mathbf{r}') = {} & \alpha[u_1(\mathbf{r})u_1^*(\mathbf{r}') - u_2(\mathbf{r})u_2^*(\mathbf{r}')]k_z \\ & + \beta[u_1(\mathbf{r})u_2^*(\mathbf{r}')k_- + u_2(\mathbf{r})u_1^*(\mathbf{r}')k_+]. \end{aligned} \tag{3}$$

The solution of the corresponding secular equation has the form

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

As to the other double-valued representation E_1' (which in the present case is a combination of two complex-conjugate one-dimensional representations), then from the corresponding basis functions one can construct only an invariant or a combination which gives an invariant together with k_z. Thus, for the energy spectrum we obtain

$$\varepsilon_{1,2} = \alpha k^2 + \beta k_z^2 \pm \gamma k_z. \tag{5}$$

In this connection a "Fermi point" cannot appear.

In the case of the group D_6 the representations E_1' and E_2' give a situation analogous to E_2' in D_3, i.e. to formula (4), and the representation E_3' is analogous to E_1' in D_3, i.e., it does not correspond to a "Fermi point." Finally, in the group D_4 both double-valued two-dimensional representations are analogous to E_2' in the group D_3 and give formula (4).

In all of the described cases of the occurrence of a "Fermi point" the fact that the basis functions permitted the construction of an invariant linear in k_z was very important. This does not hold in other point groups with one axis of high order. In these groups the component k_z may appear in the function $Q(\mathbf{k}; \mathbf{r}, \mathbf{r}')$ only in the form k_z^2. But k_z^2 is an invariant by itself, and therefore the energy spectrum will have the form

$$\varepsilon_{1,2} = \alpha k_z^2 + f_{1,2}(k_x, k_y). \tag{6}$$

Consequently the branches do not separate along the direction k_z, i.e., a "Fermi point" is impossible.

3. CUBIC GROUPS. SINGLE-VALUED REPRESENTATIONS

Let us go on to the cubic groups. We note that since the functions u_i enter by pairs, then there is no difference between even and odd representations, so that one cannot determine the parity of the representation.

The components of the vector k transform according to one of the three-dimensional representations of the cubic groups, and from the quadratic combinations one can set up the bases of three representations: the invariant k^2, the basis of a two-dimensional representation $(k_z^2 + \theta k_x^2 + \theta^2 k_y^2,\, k_z^2 + \theta^2 k_x^2 + \theta k_y^2)$ where $\theta = e^{2\pi i/3}$, and the basis of one of the three-dimensional representations $(k_x k_y,\, k_y k_z,\, k_z k_x)$.

Let the functions u_i correspond to the two-dimensional representation. By the usual method one can establish that from such functions one can make up only the invariant $u_1(\mathbf{r})u_1^*(\mathbf{r}') + u_2(\mathbf{r})u_2^*(\mathbf{r}')$ and the basis of the two-dimensional representation $u_1(\mathbf{r})u_2^*(\mathbf{r}')$, $u_2(\mathbf{r})u_1^*(\mathbf{r}')$. Owing to this we can easily determine the function $Q(\mathbf{k}; \mathbf{r}, \mathbf{r}')$ (see[5]) and find an expression for the energy levels

$$\varepsilon_{1,2} = \alpha k^2 \pm \beta[k^4 - 3(k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)]^{1/2}. \tag{7}$$

Having taken k in the [111] direction we obtain $\epsilon_{1,2} = \alpha k^2$, from which it follows that although degeneracy occurs at the point k = 0 it does not simultaneously correspond to a minimum of one of the functions $\epsilon_i(\mathbf{k})$ and a maximum of the other.

Let us go on to the three-dimensional representations. Here it is easiest of all to follow the method indicated in[6] (see also[8]). The bilinear combinations of interest to us are $u_i^*(\mathbf{r}')[f(\hat{J})]_{ik}u_k(\mathbf{r})$, where $f(\hat{J})$ is some kind of product of the spin projection operators (in the present case J = 1). These combinations transform in the same way as the operators $f(\hat{J})$ themselves, and therefore it is necessary for us in turn to construct invariants out of the components of k and of the operators $\hat{J}$. Since J = 1 the invariants may be either linear or quadratic in $\hat{J}$. From the requirement of invariance under time reversal it follows that the total power of k and $\hat{J}$ should be even.

If the little group of k is equivalent to the group T or O, then an invariant exists which is linear in k, namely, the product $\mathbf{k}\cdot\hat{\mathbf{J}}$. Confining our attention to this approximation we obtain

$$\varepsilon_{1,2,3} = +vk, \quad 0, \quad -vk. \tag{8}$$

For the final solution of the question about whether the point k = 0 possesses the necessary properties, it is necessary to determine whether it corresponds to an extremum of the function $\epsilon_2(\mathbf{k})$. For this it is necessary to find the next approximation for $\epsilon_2(\mathbf{k})$. Among the invariants is αk^2, and one can assume that it is larger than all remaining invariants. In this connection, the function $\epsilon_2(\mathbf{k})$ will have the same sign for all values of k. Therefore, in the present case the point k = 0 may correspond to contact of the conduction band with the valence band.

In the case when the little group is equivalent to T_h or O_h, i.e., when it contains a center of inversion, the invariants must necessarily contain an even number of k and an even number of $\hat{J}$. The same pertains in the present case to the group T_d, although it does not contain a center of inversion. This is related to the fact that the scalar product $(\mathbf{k}\cdot\hat{\mathbf{J}})$ is not an invariant for this group, but the invariants which are linear in k and cubic in $\hat{J}$ are absent for J = 1. One can show that in all three groups there is one and the same common invariant:

$$\begin{aligned} \hat{D} = {} & \alpha k^2 + \beta[(J_z^2 + \theta J_x^2 + \theta^2 J_y^2)(k_z^2 + \theta^2 k_x^2 + \theta k_y^2) \\ & + (J_z^2 + \theta^2 J_x^2 + \theta J_y^2)(k_z^2 + \theta k_x^2 + \theta^2 k_y^2)] \\ & + \gamma[k_x k_y\{J_x, J_y\} + k_y k_z\{J_y, J_z\} + k_z k_x\{J_z, J_x\}], \end{aligned} \tag{9}$$

where $\{J_x, J_y\} = J_x J_y + J_y J_x$. The corresponding secular equation has the form

$$(\varepsilon-\alpha k^2)^3-(\varepsilon-\alpha k^2)[3\beta^2k^4+(\gamma^2-9\beta^2)(k_x^2k_z^2+k_y^2k_z^2+k_x^2k_y^2)]+2\beta^3k^6+\beta(\gamma^2-9\beta^2)k^2(k_x^2k_z^2+k_y^2k_z^2+k_y^2k_x^2)-(2\gamma^3-9\beta\gamma^2-9\beta^3)k_x^2k_y^2k_z^2=0. \tag{10}$$

Let us demonstrate that the coefficients α, β, and γ can be chosen in such a way that the eigenvalues $\epsilon_i(\mathbf{k})$ will have different signs, where each of them will retain its sign for all directions **k**. The determinant of the matrix D_{ik} given by Eq. (9) is the product of the three functions $\epsilon_1(\mathbf{k})\epsilon_2(\mathbf{k})\epsilon_3(\mathbf{k})$. If one of them changes sign for any value of k, then the determinant must vanish at this point. Hence one of the conditions is $\|D_{ik}(\mathbf{k})\| \neq 0$. For this it is obviously necessary that all extrema of $\|D_{ik}(\mathbf{k})\|$ as a function of the direction of k do not vanish and have one and the same sign. But the extrema of the determinant correspond to the most symmetric directions, namely [100], [110], and [111]. Therefore, it is sufficient to establish the conditions under which, let us say, $\|D_{ik}\| < 0$ in these three directions. In addition, it is necessary that in one of the indicated directions the functions $\epsilon_i(\mathbf{k})$ have different values, i.e., for example, for $\|D_{ik}\| < 0$ the values $\epsilon_1 < 0$ and $\epsilon_2, \epsilon_3 > 0$. The condition that there be one negative function and two positive functions $\epsilon_i(\mathbf{k})$ for all three symmetric directions of **k** is obviously equivalent to these requirements.

For such directions the functions $\epsilon_i(\mathbf{k})$ can easily be found:

$$
\begin{aligned}
&[100]: && \varepsilon_1=(\alpha-2\beta)k^2, && \varepsilon_2=\varepsilon_3=(\alpha+\beta)k^2,\\
&[110]: && \varepsilon_1=[\alpha-{}^1/_2(\beta+\gamma)]k^2, && \varepsilon_2=[\alpha-{}^1/_2(\beta-\gamma)]k^2,\ \varepsilon_3=(\alpha+\beta)k^2\\
&[111]: && \varepsilon_1=[\alpha-{}^2/_3\gamma]k^2, && \varepsilon_2=\varepsilon_3=(\alpha+{}^1/_3\gamma)k^2.
\end{aligned} \tag{11}
$$

It is not difficult to show that ranges of the values of α, β, and γ exist in which $\epsilon_1 < 0$ and $\epsilon_2, \epsilon_3 > 0$. Thus, contact of the conduction band with the valence band is possible in the groups T_d, T_h, and O_h.

4. CUBIC GROUPS. DOUBLE-VALUED REPRESENTATIONS

Let us go on to double-valued representations. There are two kinds of such representations: two-dimensional corresponding to J = 1/2 and four-dimensional corresponding to J = 3/2. If the little group k = 0 is equivalent to T or O then again the invariant $\mathbf{k}\cdot\hat{\mathbf{J}}$ exists. For two-dimensional representations we obtain

$$\varepsilon_1=vk,\quad \varepsilon_2=-vk. \tag{12}$$

One cannot consider two-dimensional representations of the remaining groups. In fact, in the presence of a center of inversion in the lattice, the two-fold degeneracy is retained for arbitrary k, which corresponds to the fact that the energy does not depend on the direction of the spin. As for the group T_d, then here, just as for the single-valued three-dimensional representations, the necessary invariant which is linear in k is absent. Therefore, in the present case the fundamental invariant will simply be αk^2, i.e., the two functions $\epsilon_{1,2}(\mathbf{k})$ coincide in this approximation. This degeneracy is lifted only by small terms which are cubic in k, from which it is clear that in the present case the point k = 0 does not possess the required properties.

Let us go on to four-dimensional representations. In the absence of a center of inversion (T, T_d, or O) the admissible invariants can be linear in k and cubic in **J**. For the group T the general form of the invariant is given by

$$\hat{D}=\alpha(\mathbf{k}\hat{\mathbf{J}})+\beta(k_xJ_x^3+k_yJ_y^3+k_zJ_z^3)+\gamma[k_x\{J_x,(J_y^2-J_z^2)\}+k_y\{J_y(J_z^2-J_x^2)\}+k_z\{J_z,(J_x^2-J_y^2)\}], \tag{13}$$

where $\{A, B\} = AB + BA$.

In the group O the last invariant is absent, i.e., $\gamma = 0$, and in the group T_d, $\alpha = \beta = 0$. The possible existence of a "Fermi point" in the groups T and O is determined by the following simple consideration. Let $\alpha \gg \beta, \gamma$. In this case $\epsilon_1 = -(3/2)\alpha k$, $\epsilon_2 = -(1/2)\alpha k$, $\epsilon_3 = (1/2)\alpha k$, and $\epsilon_4 = (3/2)\alpha k$. Here k = 0 possesses the required properties. Hence it follows that ranges of values of the coefficients exist for which the point k = 0 retains these properties.

The group T_d is in a special position. The solution of the secular equation leads to the following eigenvalues:

$$\varepsilon_{1,2,3,4}=\pm\gamma\sqrt{3}k[1\pm\sqrt{3}/_2\sqrt{1-(n_x^4+n_y^4+n_z^2)}], \tag{14}$$

where n denotes a unit vector in the direction **k**. In the direction [111] two of the roots vanish in this approximation. In analogy to the preceding discussion, by adding the invariant δk^2 one can also verify here that the point k = 0 can possess the necessary properties. In the case when the little group contains a center of inversion (T_h or O_h), the invariant must be quadratic in **k** and **J**. The general form of the invariant is again given by formula (9). Here, however, the matrix J_i corresponds to J = 3/2. Solving the secular equation we obtain the well-known formula

$$\varepsilon_{1,2}=\alpha k^2\pm[9\beta^2k^4\pm3(\gamma^2-9\beta^2)(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{1/2}. \tag{15}$$

Each level is doubly degenerate. For the symmetric directions we obtain

$$
\begin{aligned}
&[100]: && \varepsilon_{1,2}=(\alpha\pm3\beta)k^2,\\
&[110]: && \varepsilon_{1,2}=(\alpha\pm{}^1/_2\sqrt{9\beta^2+3\gamma^2})k^2,\\
&[111]: && \varepsilon_{1,2}=(\alpha\pm\gamma)k^2.
\end{aligned} \tag{16}
$$

From here it follows that contact of the valence band and the conduction band can actually occur at the point **k** = 0. We note that precisely this representation is realized in α-Sn (usually denoted by Γ_8.

5. MORE COMPLICATED SYMMETRY

The analysis carried out above exhausts all cases involving the appearance of a "fermi point" with a little group equivalent to a point group. We shall not give such a complete analysis of the cases of more complicated symmetry, and we only show that here "Fermi points" can also appear. The appearance of nontrivial screw axes and glide planes frequently increases the multiplicity of the degeneracy of the energy levels. In the literature this phenomena is sometimes called coalescence of the energy bands. It is essential that in the majority of the cases the bands coincide on intact pieces of the surface of the Brillouin zone, and consequently there cannot be any "Fermi points" here. However, in a number of cubic groups (namely O^8 and O^{10}, and also O_h^{10}, using the notation from[9]) the little groups of the vectors $\mathbf{k}_0$ with a point at a corner of the cubic Brillouin zone have four-dimensional and six-dimensional single-valued representations.

Let us present the invariant for the four-dimensional representations:

$$
\begin{aligned}
Q(\mathbf{k};\mathbf{r},\mathbf{r}')=iv[&\{u_1(\mathbf{r})u_2^*(\mathbf{r}')-u_2(\mathbf{r})u_1^*(\mathbf{r}')\}k_z\\
&+\{u_2(\mathbf{r})u_3^*(\mathbf{r}')-u_3(\mathbf{r})u_2^*(\mathbf{r}')\}k_x+\{u_3(\mathbf{r})u_1^*(\mathbf{r}')-u_1(\mathbf{r})u_3^*(\mathbf{r}')\}k_y\\
&+\{u_3(\mathbf{r})u_4^*(\mathbf{r}')-u_4(\mathbf{r})u_3^*(\mathbf{r}')\}k_z+\{u_4(\mathbf{r})u_2^*(\mathbf{r}')-u_2(\mathbf{r})u_4^*(\mathbf{r}')\}k_y\\
&+\{u_1(\mathbf{r})u_4^*(\mathbf{r}')-u_4(\mathbf{r})u_1^*(\mathbf{r}')\}k_x].
\end{aligned} \tag{17}
$$

The matrix $\hat{D}$ may be written in the form $\hat{D}(\mathbf{k}) = v\alpha\mathbf{k}$, where the matrices α_i possess the commutation relations of the Dirac matrices. In our approximation the levels remain doubly degenerate and $\epsilon_{1,2}(\mathbf{k}) = \pm vk$.

The six-dimensional representations also admit realization of a point Fermi surface but, as in the case of three-dimensional representations of the simple cubic groups, part of the energy bands begins with terms which are quadratic in k.

Thus, we have shown that cases when contact of the valence band with the conduction band occurs in the electron spectrum are not unusual, and consequently such substances may be encountered in nature. Of course, we did not exhaust all possible cases involving complicated symmetry, but here it is apparently reasonable to consider specific examples for which the experimental data will indicate the existence of a "Fermi point."

Our conclusions have been reached in the one-electron approximation, i.e., we have not taken the interaction of the electrons into consideration. This problem merits very serious attention because it is quite possible that it may turn out that the interaction leads to instability of the obtained spectrum.

6. COULOMB INTERACTION ASSOCIATED WITH A LINEAR SPECTRUM

We consider, first of all, the simplest case of two energy branches which are described by formula (12). In this case the matrix D can be written in the form

$$\hat{D}=v(\sigma\mathbf{k}), \tag{18}$$

where the σ_i are the Pauli matrices. In accordance with this the Green's function for noninteracting electrons may be written in the form

$$G_0=[\omega-v(\sigma\mathbf{k})+i\delta\,\mathrm{sign}\,\omega]^{-1}. \tag{19}$$

Now let us introduce the Coulomb interaction between the electrons, which we shall write in the usual form. Let us consider how screening occurs. The screening interaction has the form

$$\Gamma(\mathbf{k},\omega)=\frac{4\pi e^2}{\varepsilon_0k^2-4\pi e^2\Pi(\mathbf{k},\omega)}, \tag{20}$$

where $\Pi(\mathbf{k}, \omega)$ denotes the sum of all possible electron loops. In the first approximation

$$\Pi(\mathbf{k},\omega)=-i\,\mathrm{Sp}\int\hat{G}_0(\omega_1,\mathbf{k}_1)\hat{G}_0(\omega+\omega_1,\mathbf{k}+\mathbf{k}_1)\frac{d\omega_1\,d^3k_1}{(2\pi)^4}.$$

Substituting here the function $\hat{G}_0$, which it is more convenient to write in the form

$$\hat{G}_0=\frac{\omega+v\sigma\mathbf{k}}{\omega^2-(vk-i\delta)^2}, \tag{19$'$}$$

we obtain

$$\Pi_0=-\frac{k^2}{12\pi^2v}\ln\frac{k_{max}}{\sqrt{k^2-\omega^2/v^2}}, \tag{21}$$

where k_{max} is the limit of integration, which is of the order of the period of the reciprocal lattice.

Thus, in the case under consideration the Coulomb interaction is practically not screened. As we see below, the evaluation of the self-energy corrections to the electronic spectrum with the aid of formula (20) also leads to a logarithmic integral. From here it follows that at the point **k** = 0 the energy spectrum has a singularity, and the matrix D cannot be expanded in a series in powers of **k**. However, in view of the fact that the singularity is weak, we may, without violating the symmetry conditions, assume that the matrix $\hat{D}$ is multiplied by a slowly varying invariant function, i.e., by a function which depends on the absolute value of k and on ω. In order to find this function we apply the method of article[10].

The equation for the Green's function is written in the form

$$G^{-1}=G_0^{-1}-\Sigma=\omega-v(\sigma\mathbf{k})-\Sigma(\mathbf{k},\omega). \tag{22}$$

We shall seek the complete Green's function in the form

$$G=\frac{\omega+v(\sigma\mathbf{k})f(k,\omega)}{\omega^2-[vkf(k,\omega)-i\delta]^2}, \tag{23}$$

where f is a slowly varying function of **k** and ω. The first approximation for the polarization operator, evaluated with the aid of this function instead of (19′), is

$$\Pi(\mathbf{k},\omega)=-\frac{k^2}{12\pi^2v}\int_0^{\xi}\frac{d\xi_1}{f(\xi_1)}, \tag{24}$$

where ξ is a logarithmic variable;

$$\xi=\ln\frac{k_{max}}{\max(k_1\omega/v)},\quad \xi_1=\ln\frac{k_{max}}{k_1}$$

(the integral is taken over the region where $\omega_1 \sim vk_1$). Consequently, according to (20),

$$\Gamma(\mathbf{k},\omega)=\frac{4\pi e^2}{\varepsilon_0(k^2)}d(\mathbf{k},\omega),\quad d(\mathbf{k},\omega)=\left[1+\frac{e^2}{3\pi v\varepsilon_0}\int_0^{\xi}\frac{d\xi_1}{f(\xi_1)}\right]^{-1}. \tag{25}$$

In general, besides the simplest loops of two Green's functions, more complicated diagrams (Fig. 1) enter into Π. One can join all of them together into a diagram of the first type, but in this connection one of the triple-vertices is replaced by the appropriate total vertex. For simplicity we make the assumption: $k \gtrsim \omega/v$. The logarithmic integral in Π goes over the region $\omega/v \sim k_1 \gg k$. Consequently the triple-vertex $\gamma(\mathbf{k}, \mathbf{k}_1)$ is necessary for us for $k \ll k_1$. Since the interaction is assumed to be weak, we are interested in terms containing the maximum power of the logarithm for a given power of the coupling constant. Considering the first correction to γ, we actually obtain terms with logarithmic integrals. They have the form

$$\frac{k^2}{k_1^2}d(k_1)\int_{\eta}^{\xi}\frac{d\xi_1}{f(\xi_1)}\quad\text{or}\quad\frac{\omega\sigma\mathbf{k}}{vk_1^2}d(k_1)\int_{\eta}^{\xi}\frac{d\xi_1}{f(\xi_1)};$$

$$\xi=\ln\frac{k_{max}}{k},\quad \eta=\ln\frac{k_{max}}{k_1}.$$

But upon substitution of these expressions into the integral:

$$\Pi^{(1)}=-i\,\mathrm{Sp}\int G(\mathbf{k}_1,\omega_1)G(\mathbf{k}_1+\mathbf{k},\omega_1+\omega)\gamma(\mathbf{k}\omega,\mathbf{k}_1\omega_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}$$

we obtain a convergent integral instead of a logarithmically divergent one. Therefore, the corrections to the obtained form of Π will be small, and one can neglect them.

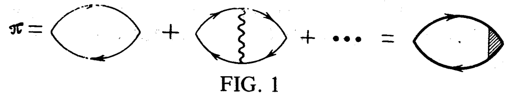

FIG. 1

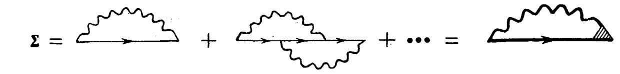

FIG. 2

Now let us go on to the self-energy of an electron. In the first approximation we have

$$\hat{\Sigma}(\omega, \mathbf{k}) = i\int \Gamma(-\omega_1, -\mathbf{k}_1)\hat{G}(\omega_1+\omega, \mathbf{k}_1+\mathbf{k})\frac{d^3k_1\,d\omega_1}{(2\pi)^4}.$$

By means of a renormalization of the chemical potential we can always eliminate an arbitrary constant from Σ. Therefore we subtract Σ(0, 0) and as a result we obtain

$$\Sigma(\omega, \mathbf{k}) = i\int [\hat{G}(\omega_1+\omega, \mathbf{k}_1+\mathbf{k}) - \hat{G}(\omega_1, \mathbf{k}_1)]\Gamma(-\omega_1, -\mathbf{k}_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}. \tag{26}$$

Aside from this term, the total self-energy contains terms corresponding to more complicated diagrams (see Fig. 2), but one can show that they give a small contribution. In fact, let us consider the next correction containing two Γ-lines. In order for this term to be important, it must contain two logarithmic integrals with respect to the momenta of the Γ-lines: k_1 and k_2. Consequently there should be two logarithmic regions, $k_1 \gg k_2 \gg k$ and $k_2 \gg k_1 \gg k$, but as already mentioned earlier the vertex γ may contain logarithmic integrals only in that case if its arguments differ appreciably in magnitude, where these integrals correspond to the regions between the values of the arguments. In view of this, in the region $k_1 \gg k_2 \gg k$ the logarithmic integral with respect to k_1 is not present, but in the second region there is no logarithmic integral with respect to k_2. Thus, we may confine our attention to expression (26). Substituting expressions (23) and (25) here, we find

$$\Sigma = \frac{2e^2}{3\pi\varepsilon_0}\sigma\mathbf{k}\int_0^{\xi} d\xi_1\, d(\xi_1). \tag{27}$$

Here $\xi_1 = \ln(k_{\max}/k_1)$, $\xi = \ln(k_{\max}/k)$, and it is assumed that $vk \gtrsim \omega$. In the case when $vk \ll \omega$,

$$\Sigma = \frac{2e^2}{3\pi\varepsilon_0}\sigma\mathbf{k}\left[\int_0^{\eta} d\xi_1\, d(\xi_1) + d(\eta)(\xi-\eta)\right], \tag{27'}$$

where $\eta = \ln(vk_{\max}/\omega)$ and $\xi = \ln(k_{\max}/k)$. The most interesting case is $\omega \sim vk$, i.e. formula (27). It is necessary to explicitly specify the case $\omega \approx \pm vk$. Strictly speaking, at such values of ω a singularity must appear in Σ because the spectrum linear in k is unstable with respect to the decay of quasi-particles into many other particles traveling in the same direction. Such singularities actually exist, but they appear only in the next approximation, in terms proportional to

$$\frac{e^4}{\varepsilon_0^2}\ln\frac{(vk_{max})^2}{(vk)^2-\omega^2}.$$

In those terms which we are considering, the lower limit of the integrals is simply k, and the proximity of ω to ±vk does not manifest itself in any way. Thus, in the approximation under consideration the case $\omega \approx \pm vk$ is described by formula (27).

If formulas (22), (23), (25), and (27) are compared, then we obtain an equation for the function f(ξ) (we assume $vk \gtrsim \omega$)

$$f(\xi) = 1 + \frac{2e^2}{3\pi v\varepsilon_0}\int_0^{\xi}\left[1 + \frac{e^2}{3\pi v\varepsilon_0}\int_0^{\xi_1}\frac{d\xi_2}{f(\xi_2)}\right]^{-1} d\xi_1. \tag{28}$$

By means of two differentiations this equation reduces to a differential equation. Solving the latter equation we obtain

$$f(\xi) = \left(1 + \frac{e^2}{\pi v\varepsilon_0}\xi\right)^{2/3} \tag{29}$$

and substituting into the expression for d(ξ) we find

$$d(\xi) = \left(1 + \frac{e^2}{\pi v\varepsilon_0}\xi\right)^{-1/3}. \tag{30}$$

Thus, for the case under consideration one obtains the result that G has a pole for $\omega = \pm vkf(\xi)$. The imaginary part which determines the attenuation is small in comparison with the real part ($\mathrm{Im}\, G^{-1}/\mathrm{Re}\, G^{-1} \sim e^2/v\epsilon_0$). For momenta of the order of or smaller than $k_{\max}e^{-v\epsilon_0/e^2}$, the energy spectrum differs from a purely linear spectrum by a logarithmic factor.

We note that the sign in front of the logarithm for d(ξ) is positive, which corresponds to a weakening of the interaction in the region of small momenta and frequencies. This situation is analogous to quantum electrodynamics and may be called the "zero-charge" situation (in electrodynamics the situation involves, of course, not a decrease of the momentum but a decrease of the radius over which the interaction is smeared out, i.e., an increase of the upper limit on the logarithmically divergent integrals).

It is of interest to clarify whether this situation is common for all types of linear spectra or if it is unique only for the model under consideration. In general a sum of the invariants of k and $\hat{J}$ with arbitrary coefficients appears in the matrix $\hat{D}$. Under the influence of the interaction each of these coefficients changes into a slowly varying function. Ultimately one must obtain a system of integral equations for these functions. Let us confine our attention to such a generalization of the case under consideration, for which the matrix $\hat{D}$ contains on only one invariant of k and J, i.e., there is only one unknown function. An examination of the problem with several arbitrary invariants would be of significant interest.

In a noninteracting model the matrix $\hat{D}$ has the form $\hat{D} = \hat{v}k$. From symmetry conditions it follows that the Green's function of the electrons has the form

$$G = [\omega - \hat{v}\mathbf{k}f(k, \omega) + i\delta\,\mathrm{sign}\,\omega]^{-1}, \tag{31}$$

where f(k, ω) is an invariant function which, in analogy with the preceding discussion, we assume to be logarithmic (this is confirmed by the following calculation). Since factors of the order of unity are not important inside the logarithm, then one can assume that the invariant function f always depends only on k^2.

Let us evaluate the polarization operator Π. It is given by

$$\Pi(k, \omega) = -i\,\mathrm{Sp}\int \hat{G}(\mathbf{k}_1, \omega_1)\hat{G}(\mathbf{k}_1+\mathbf{k}, \omega_1+\omega)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}.$$

Let us assume that the integral runs over the region $k_1 \geq k$. In the first approximation one could neglect k. However, if this is done, then the integral turns out to be equal to zero. In fact, if the trace is taken with respect to the eigenfunctions of the operator $\hat{D}(k_1)$, then we obtain the integral

$$\int\sum_i [\omega - \varepsilon_i(k) + i\delta\,\mathrm{sign}\,\varepsilon_i]^{-2}\, d\omega,$$

which is equal to zero, since the poles always lie on one side.

In view of this fact, it is necessary to use the next terms of the expansion in powers of **k**. A nonvanishing contribution can appear only from terms of the second order in **k**. It has the form

$$\Pi(\mathbf{k}, \omega) = -i\,\mathrm{Sp}\int \hat{G}(\mathbf{k}_1, \omega_1)\hat{G}(\mathbf{k}_1, \omega_1+\omega)\hat{\mathbf{v}}_1\mathbf{k} \times \hat{G}(\mathbf{k}_1, \omega_1+\omega)\hat{\mathbf{v}}_1\mathbf{k}\hat{G}(\mathbf{k}_1, \omega_1+\omega)f^2(\mathbf{k}_1, \omega_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}, \tag{32}$$

where $\hat{\mathbf{v}}_1 = \partial D(\mathbf{k}_1)/\partial\mathbf{k}_1$. Having taken the trace with respect to the eigenfunctions of the operator $\hat{D}(\mathbf{k}_1)$, we obtain

$$\Pi(\mathbf{k}, \omega) = -i\sum\int [\omega_1 - \varepsilon_i(\mathbf{k}_1) + i\delta\,\mathrm{sign}\,\varepsilon_i]^{-1}[\omega_1 + \omega - \varepsilon_1(\mathbf{k}_1) + i\delta\,\mathrm{sign}\,\varepsilon_i]^{-1} \times (\hat{\mathbf{v}}, k)_{il}[\omega_1 + \omega - \varepsilon_l(\mathbf{k}_1) + i\delta\,\mathrm{sign}\,\varepsilon_l]^{-1}(\hat{\mathbf{v}}_1\mathbf{k})_{li}\cdot \times (\omega_1 + \omega - \varepsilon_i(\mathbf{k}_1) + i\delta\,\mathrm{sign}\,\varepsilon_i)^{-1}f^2(k_1, \omega_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}.$$

Since $\hat{\mathbf{v}}_1$ is a self-adjoint operator, then $(\hat{\mathbf{v}}_1\cdot\mathbf{k})_{il}(\hat{\mathbf{v}}_1\cdot\mathbf{k})_{li} = |(\hat{\mathbf{v}}_1\cdot\mathbf{k})_{il}|^2$. In order for the integral to be different from zero, it is necessary that the poles ϵ_i and ϵ_l should have different signs. Carrying out the integration over ω_1 and assuming $\epsilon_i(k_1) - \epsilon_l(k_1) \gg \omega$, we obtain

$$\Pi(\mathbf{k}, \omega) = -2\int\sum_{\substack{v_i>0\\ v_l<0}}(v_{1i} - v_{1l})^{-3}|(\hat{\mathbf{v}}_1\mathbf{k})_{il}|^2 f^{-1}(k_1)\frac{d^3k_1}{k_1^3(2\pi)^3}.$$

(Here we have introduced the notation $\epsilon_i(k_1) = v_{1i}k_1f(k_1)$, i.e., $v_{1i}(\mathbf{n})$ is the coefficient in the appropriate branch of the energy spectrum, and **n** is a unit vector in the direction of $\mathbf{k}_1$.) Introducing logarithmic variables we obtain

$$\Pi(\mathbf{k}, \omega) = -\frac{1}{\pi^2}\overline{\sum_{\substack{v_{1i}>0\\ v_{1l}<0}}(v_{1i} - v_{1l})^{-3}|(\hat{\mathbf{v}}_1\mathbf{k})_{il}|^2}\int_0^{\xi}\frac{d\xi_1}{f(\xi_1)},$$

where the bar denotes averaging over the directions of k_1. The function Γ will have the form

$$\Gamma = \frac{4\pi e^2}{\varepsilon_0 k^2}d(\xi), \qquad d(\xi) = \left[1 + a\int_0^{\xi}\frac{d\xi_1}{f(\xi_1)}\right]^{-1}, \tag{33}$$

$$a = \frac{4e^2}{\pi\varepsilon_0}\overline{\sum_{\substack{v_{1i}>0\\ v_{1l}<0}}(v_{1i} - v_{1l})^{-3}\left|\left(\frac{\hat{v}_1k}{k}\right)_{il}\right|^2}. \tag{34}$$

In the same way as earlier, one can show that the corrections of higher order in e^2 are small.

Let us go on to the self-energy. In analogy to the previous discussion, it is sufficient to consider only the first diagram. Since the integral over k_1 is logarithmic, then we may expand the difference $\hat{G}$ in the integral (26) with respect to k. Having made use of the fact that Γ is an even function of **k** and ω, we obtain

$$\hat{\Sigma}(\omega, \mathbf{k}) = i\int\left[\hat{G}(\omega_1, \mathbf{k}_1)\hat{\mathbf{v}}_1\mathbf{k}\hat{G}(\omega_1, \mathbf{k}_1)\cdot f(k_1, \omega_1)\Gamma(\omega_1, \mathbf{k}_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}\right].$$

From considerations of symmetry it follows that $\Sigma \sim \hat{\mathbf{v}}\cdot\mathbf{k}$. According to formula (31), $\hat{\Sigma} = \hat{\mathbf{v}}\cdot\mathbf{k}(f-1)$. Having substituted this expression, we multiply by $\hat{\mathbf{v}}\mathbf{k}$ and take the trace on both sides. In this connection we obtain

$$\sum_{i,l}|(\hat{\mathbf{v}}\mathbf{k})_{il}|^2[f(\xi) - 1] = i\sum_{i,l}\int(\hat{\mathbf{v}}_1\mathbf{k})_{il}(\omega - \varepsilon_i + i\delta\,\mathrm{sign}\,\varepsilon_i)^{-1} \times (\hat{\mathbf{v}}_1\mathbf{k})_{il}(\omega - \varepsilon_l + i\delta\,\mathrm{sign}\,\varepsilon_l)^{-1}f(k_1)\Gamma(\omega_1, k_1)\frac{d^3k_1\,d\omega_1}{(2\pi)^4}$$
$$= 2\int\sum_{\substack{v_{1l}>0\\ v_{1i}<0}}|(\hat{v}_1k)_{il}|^2(v_{1i} - v_{1l})^{-1}\frac{1}{k_1}\frac{4\pi e^2}{\varepsilon_0 k_1^2}d(k_1)\frac{d^3k_1}{(2\pi)^3}.$$

Carrying out the last integration, we obtain the relation

$$f(\xi) = 1 + b\int_0^{\xi} d(\xi_1)\, d\xi_2, \tag{35}$$

where

$$b = \frac{4e^2}{\pi\varepsilon_0}\sum_{\substack{v_{1i}>0\\ v_{1l}<0}}\left|\left(\frac{\hat{\mathbf{v}}_1\mathbf{k}}{k}\right)_{il}\right|^2(v_{1i} - v_{1l})^{-1}\left(\sum_{i,l}\left|\left(\frac{\hat{\mathbf{v}}\mathbf{k}}{k}\right)_{il}\right|^2\right)^{-1}. \tag{36}$$

Equations (33) and (35) differ from (28) only by the coefficients. The solution has the form

$$f(\xi) = [(a+b)\xi + 1]^{a/(a+b)}, \tag{37}$$

$$d(\xi) = [(a+b)\xi + 1]^{-b/(a+b)}. \tag{38}$$

According to the definitions (34) and (36), both coefficients a and b are positive and of the order of $e^2/v\epsilon_0$. Thus, the conclusions reached for the simplest example considered at the beginning are completely valid for the more general case of a "Fermi point" with a linear spectrum.

7. QUADRATIC SPECTRUM

The situation is completely different in the case of a quadratic spectrum. First of all we note that if we set k = 0 in the polarization operator, then we obtain zero independently of the form of the spectrum. A nonvanishing contribution appears in second order in k. But in the present case the integral analogous to (32) is convergent and for $\omega \ll k$ has the form mk, where m is the order of the mass of a free electron. Therefore the function **Γ** will have the form

$$\Gamma = 4\pi e^2/(\varepsilon_0 k^2 + me^2ka),$$

where a ~ 1. Thus, for $k < me^2/\epsilon_0$ the behavior of Γ changes radically. One can use the obtained expression in order to evaluate the following corrections to the triple-vertex γ.

Let us consider the first such correction (Fig. 3). The corresponding expression has the form

$$\gamma(\mathbf{k}_1, \omega_1; \mathbf{k}_1+\mathbf{k}, \omega_1+\omega) = \int\hat{G}(\mathbf{k}_2, \omega_2)\hat{G}(\mathbf{k}_2+\mathbf{k}, \omega_2+\omega)\Gamma(\mathbf{k}_1-\mathbf{k}_2, \omega_1-\omega_2)\frac{d^3k_2\,d\omega_2}{(2\pi)^4}.$$

We shall assume $k_1 \gg k$, and we shall use a representation which diagonalizes $D(k_1)$. However since $\hat{G}(k_2)$ stands inside the integral, then we arrive at a representation which diagonalizes $D(k_2)$ by introducing conversion coefficients $C_{il}(k_1k_2)$. If we assume $k_2 \gg k$, then in the first approximation one can neglect k inside the integral. But in this connection we obtain

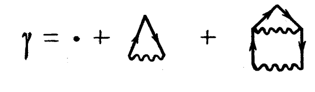

FIG. 3

$$\int \sum_n C_{in}(k_1k_2)\,(\omega_2-\varepsilon_n(k_2)+i\delta\,\mathrm{sign}\,\varepsilon_n)^{-1}$$
$$\times(\omega_2+\omega-\varepsilon_n(k_2)+i\delta\,\mathrm{sign}\,\varepsilon_n)^{-1}C_{nl}(k_2k_1)\frac{d\omega_2}{2\pi}.$$

In each of the terms of the sum, the poles with respect to ω_2 lie on the same side of the real axis. Therefore the corresponding integral is equal to zero. A finite contribution appears only in first order with respect to **k**. This introduces an extra factor k/k_2 into the integrand. After this one can easily see that the integral will converge, and in the region $k < me^2/\epsilon_0$ it turns out that $\gamma^{(1)} \sim 1$. One can verify that this is valid for the corrections to γ of arbitrary order.

Here we encounter a new situation: at small momenta all of the terms of the perturbation-theoretic series become of the same order, i.e., weak coupling changes into strong coupling. Such a situation also arises in certain versions of field theory, and also in the problem of a phase transition of the second kind. This situation was considered in the well-known work by V. N. Gribov and A. A. Migdal,[11] where it was shown that the behavior of the fundamental quantities is determined by power laws which are established with the aid of the theory of scaling. We shall use the method of article[11].

We make the assumption that the dependence of all quantities on k and ω is determined by the following relations (we do not present the detailed matrix structure, which depends on the specific representation):

$$G=c_1k^{-\alpha}g(\omega/sk^\nu),\qquad \gamma=c_2k^\beta q(\omega/sk^\nu),\qquad \Gamma=c_3k^{-\delta}d(\omega/sk^\nu), \tag{39}$$

and we choose the powers α, β, δ, ν and the constants c_1, c_2, c_3, and s in order to satisfy all the relations of the theory (here a symmetric γ is to be understood, i.e., having arguments of the same order).

First of all, on the basis of the previous discussion one can conclude that for small momenta $4\pi e^2\Pi \gg \epsilon_0k^2$ and $\Sigma \gg G_0^{-1}$, i.e., the behavior of the G- and Γ-functions is determined by the self-energy parts. But the corresponding integrals only depend on k if k is sufficiently large, and they only depend on ω if ω dominates. This is guaranteed only in that case when in (39)

$$\begin{aligned} g(0)&=1, & g(x\gg1)&\sim x^{-\alpha/\nu},\\ q(0)&=1, & q(x\gg1)&\sim x^{\beta/\nu},\\ d(0)&=1, & d(x\gg1)&\sim x^{-\delta/\nu}\end{aligned} \tag{40}$$

(the values at zero are normalized by the appropriate choice of the constant).

Let us consider the diagrams of higher orders for γ. The transition to the next order means the appearance in the diagram of two additional G-lines, two γ vertices, one Γ-line, and integration over $d^3k\,d\omega$. We require that this operation preserve the form of γ. For this it is necessary that

$$\int G^2\gamma^2\Gamma\,d^3k_1\,d\omega_1 \sim 1.$$

Substituting (22) and proceeding to the integration with respect to $x_1 = \omega/sk_1^\nu$, from here we obtain

$$c_1^2c_2^2c_3sk^{-2\alpha+2\beta-\delta+\nu+3}\int g^2q^2\,d\,dx \sim 1.$$

Hence it follows that

$$-2\alpha+2\beta-\delta+\nu+3=0, \tag{41}$$

$$c_1^2c_2^2c_3s \sim 1. \tag{42}$$

Here it is necessary to add a condition in order that the integral in the correction for γ should converge. Considering the first correction, but with complete lines and vertices, we obtain

$$-2\alpha+3\beta-\delta+\nu+3<0. \tag{43}$$

This guarantees the convergence of the integral over k. It is not difficult to see that here the integral over x will automatically converge.

Then let us consider the G-function. First of all we note that it satisfies the so-called Ward identity:

$$\partial G^{-1}/\partial\omega=\gamma. \tag{44}$$

Substituting formula (39) here, we obtain

$$sc_1c_2k^{\beta-\alpha+\nu} \sim 1,$$

from where it follows that

$$\beta-\alpha+\nu=0, \tag{45}$$

$$sc_1c_2 \sim 1. \tag{46}$$

Now we introduce a new function[1)] γ_2 which we define as

$$\gamma_2=\partial^2G^{-1}/\partial k^2. \tag{47}$$

We assume that this function has a form analogous to (39), that is,

$$\gamma_2=c_4k^\mu\varphi(\omega/sk^\nu). \tag{48}$$

Substituting (39) and (48) into relation (47), we obtain

$$\mu-\alpha+2=0, \tag{49}$$

$$c_4c_1 \sim 1. \tag{50}$$

Now let us consider $\Sigma(\mathbf{k},\omega)-\Sigma(0,0)$. In the expansion in terms of k in the integral for the self-energy, the contribution of second order in **k** is essential. Taking into consideration that according to our condition all of the diagrams give a contribution of the same order of magnitude, it is sufficient to consider only the first diagram (Fig. 4). From it we obtain ($\omega \ll sk^\nu$)

$$\Sigma(\mathrm{k},\omega)-\Sigma(0,0) \sim k^2\int G^2\gamma_2\gamma^2\Gamma\,d^3k_1\,d\omega_1.$$

If this expression is assumed to be of order G^{-1}, then conditions (41) and (42) are again obtained here together with (49) and (50). From this point of view the introduction of the quantity γ_2 does not give anything new. It is necessary, however, so that the integral $\Sigma(\mathbf{k},\omega)-\Sigma(0,0)$ converges. Hence follows the requirement

$$3+\mu+2\beta-\delta-2\alpha+\nu>0. \tag{51}$$

Let us go on to the polarization operator. In the previous Section it was shown that in the first approximation $\Pi = 0$ for $k = 0$. In the general case it is not difficult to see that $\Pi(0, 0) = 0$. This follows from the fact that $\Pi(0, 0)$ determines the change of the number of particles due to the action of the electrostatic potential, which does not depend on the coordinates. Mathematically this is written as:

$$\Pi(0,0)=-i\int \mathrm{Sp}\,G^2(\omega_1,\mathbf{k}_1)\gamma(\omega_1,\mathbf{k}_1)\frac{d\omega_1\,d\mathbf{k}_1}{(2\pi)^4}=i\int \mathrm{Sp}\frac{\partial G}{\partial\omega_1}\frac{d\omega_1\,d\mathbf{k}_1}{(2\pi)^4}=0.$$

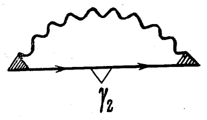

FIG. 4

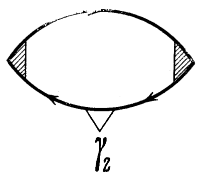

FIG. 5

Expanding the integrand up to second order in k, we obtain for $\omega \ll sk^\nu$ (see Fig. 5)

$$\Pi \sim k^2\int d^3k_1\,d\omega_1G^3\gamma_2\gamma^2.$$

Assuming $\Gamma \sim 1/\Pi$ and using (39) and (48), we again obtain the old relations for the powers and for the coefficients. However, the condition for convergence of the right hand side gives a new restriction:

$$3+\mu+2\beta+\nu-3\alpha<0. \tag{52}$$

Relations (41), (45), and (49) give the possibility to express all of the coefficients α, β, δ, μ, and ν in terms of any two of them, for example:

$$\delta=3-\nu,\qquad \beta=\alpha-\nu,\qquad \mu=\alpha-2. \tag{53}$$

From conditions (43), (51), and (52) with the aid of (53) we obtain the following restrictions on the possible values of the coefficients:

$$\nu>1,\quad \alpha<2,\quad \alpha<\nu,\quad \delta<2,\quad \beta<0,\quad \mu<0. \tag{54}$$

The question may arise whether new restrictions cannot appear if we enclose several vertices of type γ_2 and γ by Coulomb lines. If we have n_1 vertices of type γ_2 and n_2 vertices of type γ, then the condition for convergence is written in the form

$$n_1\mu+n_2\beta-\alpha(n_1+n_2-1)<0.$$

Substituting (45) and (49), we obtain

$$\alpha<2n_1+\nu n_2.$$

This condition is ensured by the inequalities (54).

It is of interest that upon fulfillment of the restrictions (54), the behavior of G and Γ for small momenta and frequencies actually is determined by the self-energy parts. For $\omega \ll sk^\nu$ this is ensured by the conditions $\alpha < 2$, $\delta < 2$, but for $\omega \gg sk^\nu$ this follows from the condition $\alpha < \nu$.

For the constants c_1, c_2, c_3, and s we have, according to (42) and (46),

$$sc_1c_2 \sim 1,\qquad c_1c_2c_3 \sim 1. \tag{55}$$

The orders of magnitude of these constants are obtained from the conditions for joining with the region of large momenta. According to the previous discussion, joining should occur for $k \sim me^2/\epsilon_0$. In the region of large momenta the electron spectrum is given by $\omega \sim k^2/m$. Therefore, with regard to ω, joining should occur for $\omega \sim me^4/\epsilon_0^2$. It is natural to expect that in the joining region $\omega \sim sk^\nu$. From here it follows that

$$s \sim (e^2/\varepsilon_0)^{2-\nu}m^{1-\nu}. \tag{56}$$

In the joining region the function Γ is of the order of $(e^2/\epsilon_0k^2) \sim (\epsilon_0/m^2e^2)$. Comparing with expression (39) we have

$$c_3 \sim (e^2/\varepsilon_0)^{\delta-1}m^{\delta-2} \sim (e^2/\varepsilon_0)^{2-\nu}m^{1-\nu}. \tag{57}$$

In the joining region the function G is of the order of $1/\omega$ or $(me^4/\epsilon_0^2)^{-1}$. Hence it follows that

$$c_1 \sim (e^2/\varepsilon_0)^{\alpha-2}m^{\alpha-1}. \tag{58}$$

Finally, for $k \sim me^2/\epsilon_0$, γ should be of the order of unity. Hence

$$c_2 \sim (me^2/\varepsilon_0)^{-\beta}. \tag{59}$$

The values (56)—(59) satisfy the relations (55).

From the obtained results it follows that in the region $k < me^2/\epsilon_0$ the electron's Green's function does not have such a simple form as for large momenta. Its poles, if such exist in general, may be complex, where in general their imaginary part is of the order of the real part. Therefore, in this region it is impossible to talk about quasi-particles in the usual sense of the word.

However, the value of the Green's function makes it possible to determine various physical effects. Of course, it is necessary to bear in mind that the theory developed above does not give the exact value of the constant, and also of the functions g, q, and d in the region $x \sim 1$. However, even what is known makes it possible to make a number of predictions.

Let us consider the momentum distribution of the particles. It is expressed by the integral

$$n(k)=-i\int_{-\infty}^{+\infty}G(\omega,\mathrm{k})\,e^{i\omega\tau}\frac{d\omega}{2\pi},$$

where $\tau \to +0$. Using formula (22) we obtain

$$n(k) \sim c_1sk^{-\alpha+\nu}\int g(x)\,dx.$$

But as $x \to \infty$ the quantity $g \sim x^{-\alpha/\nu}$ and since $\alpha < \nu$ according to what was said previously, the integral diverges. Hence for small momenta n(k) is actually determined by the value of G in the region of large momenta, and we do not have the right to use formula (22) directly. One can, however, evaluate the difference

$$n(k)-n(0) \sim -i\int_{-\infty}^{+\infty}[G(\omega,k)-G(\omega,0)]\,e^{i\omega\tau}\frac{d\omega}{2\pi}.$$

In this integral the region of large values of ω is contracted, and the integral converges for $x \sim 1$. In this connection we obtain

$$n(k)-n(0) \sim c_2sk^{\nu-\alpha} \sim (k\varepsilon_0/me^2)^{\nu-\alpha}. \tag{60}$$

According to Eq. (37) the power $\nu - \alpha$ is positive. In the region of large momenta we again obtain a constant.

Now let us consider the heat capacity at low temperatures. According to[2] we have

$$\Omega(T)-\Omega(0)=2\left(T\sum_\omega-\frac{1}{2\pi}\int d\omega\right)\int\frac{d^3k}{(2\pi)^3}e^{i\omega\tau}\ln G(\omega,k), \tag{61}$$

It is necessary to take $G(\omega)$ for $T = 0$. Replacing the summation over ω by an integration over real frequencies and differentiating with respect to T, we obtain the entropy

---

[1)] One can also introduce $\gamma_1 = \partial G^{-1}/\partial k$. However, in view of its oddness with respect to k, as the final result it will be proportional to $k\gamma_2$.

$$S(T) = -\frac{\partial\Omega}{\partial T} = -\frac{2}{\pi}\int_{-\infty}^{+\infty}\frac{\omega}{T}\frac{\partial n_F}{\partial\omega}\int\frac{d^3k}{(2\pi)^3}\,\mathrm{Im}\ln G_R(\omega, k),$$

where n_F denotes the Fermi function. It is impossible to evaluate this integral by the same method as in the presence of the Fermi surface. However, we obtain a result correct to within a constant coefficient if we assume that only small values of ω are essential. Taking into account the evenness of $\partial n_F/\partial\omega$, we obtain

$$S(T) \sim T\int\frac{d^3k}{(2\pi)^3}\left[\frac{\partial}{\partial\omega}\,\mathrm{Im}\ln G_R(\omega, k)\right]_{\omega\sim T}.$$

Regarding the imaginary part of G to be of the order of the real part, we may remove the Im sign and write the derivative inside the square brackets as

$$G(\omega, k)\frac{\partial G^{-1}(\omega, k)}{\partial\omega} = G\gamma.$$

Substituting G according to formula (22) we obtain

$$S \sim C \sim c_1c_2T\int d^3k\,k^{-\alpha+\beta}g\left(\frac{T}{sk^\nu}\right)q\left(\frac{T}{sk^\nu}\right).$$

Changing to the variable $x = T/sk^\nu$, we verify that the integral over x is convergent. Substituting the values of the coefficients c_1, c_2, and s, we finally obtain

$$C \sim \left(\frac{me^2}{\varepsilon_0}\right)^3\left(\frac{T\varepsilon_0^2}{me^4}\right)^{3/\nu}. \tag{62}$$

Taking the restriction (37) into account, we find the power of the temperature:

$$3 > 3/\nu > 0. \tag{63}$$

we note that one can also obtain the temperature dependence of the heat capacity from the following simple argument. The heat capacity is proportional to $T_\rho(T)$, where ρ is the density of the electronic states. The polarization operator Π is proportional to ρ. Therefore $\rho(T) \sim k^\delta(T)$, where k(T) denotes the momenta characteristic for a given temperature. It is obvious that $k(T) \sim T^{1/\nu}$. Also keeping in mind that $\delta = 3 - \nu$, we obtain $C \sim T^{3/\nu}$.

In conclusion the authors express their gratitude to L. P. Gor'kov, A. A. Migdal, and I. E. Dzyaloshinskiĭ for valuable discussions.

---

[1] L. D. Landau, Zh. Eksp. Teor. Fiz. 30, 1058 (1956) [Sov. Phys.-JETP 3, 920 (1957)].

[2] J. M. Luttinger, Phys. Rev. 119, 1153 (1960).

[3] Steven Groves and William Paul, Phys. Rev. Letters 11, 194 (1963).

[4] V. I. Ivanov-Omskiĭ, B. T. Kolomiets, L. I. Kleshchinskiĭ and K. P. Smekalova, Fiz. Tverd. Tela 10, 3106 (1968) [Sov. Phys.-Solid State 10, 2447 (1969)].

[5] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskiĭ, Metody kvantovoĭ teorii polya v statisticheskoĭ fizike (Methods of Quantum Field Theory in Statistical Physics), Fizmatgiz, 1962 (English Transl., Prentice-Hall, Inc., 1963).

[6] A. A. Abrikosov, Zh. Eksp. Teor. Fiz. 43, 1083 (1962) [Sov. Phys.-JETP 16, 765 (1963)].

[7] P. Nozières and J. M. Luttinger, Phys. Rev. 127, 1423 (1962); J. M. Luttinger and P. Nozières, Phys. Rev. 127, 1431 (1962).

[8] G. E. Pikus, Zh. Eksp. Teor. Fiz. 41, 1258, 1507 (1961) [Sov. Phys.-JETP 14, 898, 1075 (1962)].

[9] O. V. Kovalev, Neprivodimye predstavleniya prostranstvennykh grupp (Irreducible Representations of the Space Groups), Kiev, 1961.

[10] L. D. Landau, A. A. Abrikosov, and I. M. Khalatnikov, Dokl. Akad. Nauk SSSR 95, 1177 (1954).

[11] V. N. Gribov and A. A. Migdal, Zh. Eksp. Teor. Fiz. 55, 1498 (1968) [Sov. Phys.-JETP 28, 784 (1969)].

Translated by H. H. Nickle
148

SOVIET PHYSICS JETP VOLUME 32, NUMBER 4 APRIL, 1971

DOMAIN STRUCTURE PRODUCED IN AN ANTIFERROMAGNET WHEN THE CHARACTER OF THE MAGNETIC ANISOTROPY IS ALTERED

V. G. BAR'YAKHTAR, A. E. BOROVIK, V. A. POPOV, and E. P. STEFANOVSKIĬ

Physicotechnical Institute of the Ukrainian Academy of Sciences

Submitted April 14, 1970

Zh. Eksp. Teor. Fiz. 59, 1299–1306 (October, 1970)

We consider the temperature first-order phase transition, at which the magnetic anisotropy of the "easy axis" type goes over into magnetic anisotropy of the "easy plane" type. We investigate the distribution of the magnetic moments of the sublattices in the boundary between the two different phases, and calculate the surface energy of the separation boundary. It is shown that the phase transition can give rise to a thermodynamically-stable domain structure due to the weak ferromagnetism of the phase with the "easy-plane" magnetic anisotropy. The dimensions of the domains are calculated. We investigate also the distribution of the magnetic moments in 180° domain boundaries and calculate the surface energies of these boundaries. It is shown that the surface energy of an 180° boundary is greatly reduced when the phase-transition temperature is approached.

1. INTRODUCTION

As is well known, in a number of antiferromagnets (AFM) (for example, in α-Fe_2O_3), the character of the magnetic anisotropy changes appreciably with changing temperature, namely, above a certain temperature T_M (T_M is the Morin temperature) the magnetic moments are oriented perpendicular (parallel) to the chosen axis, and below this temperature the magnetic moments of the sublattices are parallel (perpendicular) to the chosen axis.

Such a change in the orientation of the magnetic moments, in the case of uniaxial AFM, i.e., AFM in which the anisotropy in the basal plane is small, indicates either a first-order phase transition, or the presence of at least two second-order phase transitions. Indeed, from symmetry considerations it is clear that in a uniaxial AFM there can be realized three phases in sequence: a phase $\Phi_\parallel$, in which the antiferromagnetism vector **l** is oriented parallel to the symmetry axis, a phase $\Phi_\perp$, in which the vector **l** is oriented perpendicular to the symmetry axis, and a phase $\Phi_<$, in which the vector **l** is oriented at a certain angle to the anisotropy axis. The transition from the phase $\Phi_\parallel$ to the phase $\Phi_\perp$ is of first order if these phases can coexist; the transition from the phase $\Phi_\parallel(\Phi_\perp)$ to the phase $\Phi_<$ can be regarded as a second-order phase transition, for in such a transition one of the symmetry elements is lost and one of the frequencies of the homogeneous oscillations vanishes on the transition line.

We consider in the present paper, in the main, the case of a first-order phase transition $\Phi_\parallel \rightleftarrows \Phi_\perp$. As is well known, in a first order phase transition there is coexistence of the phases, and consequently separation boundaries are produced between these phases.

In the phase $\Phi_\perp$, as a rule, there occurs a small magnetic moment due to the Dzyaloshinskiĭ interaction. The presence of the magnetic moment in the phase $\Phi_\perp$ makes it possible for the AFM sample to break up at temperatures close to T_M into domains that are thermodynamically stable. These domains are analogous to those investigated in[1], which arise when the antiferromagnetism vector **l** in an AFM with magnetic anisotropy of the "easy axis" (EA) type turns over in an external magnetic field.

We obtain in this paper the distributions of the magnetic moments of the AFM sublattices in the boundaries between the phases $\Phi_\parallel$ and $\Phi_\perp$ (90° boundaries), and also in the 180° introduction boundaries in AFM with weak ferromagnetism; we calculate the surface energies of the 90 and 180° interdomain walls, determine the domain structures (DS) for a plane-parallel plate, and estimate the domain dimensions.

2. THE PHASE TRANSITION $\Phi_\parallel \rightleftarrows \Phi_\perp$ IN AN UNBOUNDED AFM

Before we investigate the DS, let us consider the question of the phase transition $\Phi_\parallel \rightleftarrows \Phi_\perp$ in an infinite AFM. As already noted in the introduction, this transition can occur either via a first-order transition, or via two second-order phase transitions. The simplest density of the non-equilibrium thermodynamic potential, which makes it possible to describe these two possibilities, is

$$w = \frac{1}{2}\delta(\mathbf{M}_1 + \mathbf{M}_2)^2 - \frac{1}{8}\beta'(\mathbf{M}_1 - \mathbf{M}_2, \mathbf{n})^2 - \frac{1}{8}\beta(\mathbf{M}_1 + \mathbf{M}_2, \mathbf{n})^2$$
$$- \frac{1}{2}d(\mathbf{n}[\mathbf{M}_1\mathbf{M}_2]) - \frac{1}{4\cdot 16}\beta_3(\mathbf{M}_1 - \mathbf{M}_2, \mathbf{n})^4 + f\left(\frac{1}{2}M_1^2, \frac{1}{2}M_2^2\right), \tag{2.1}$$

where δ is the exchange-interaction constant, β, β', and β_3 are the magnetic-anisotropy constants, d is the Dzyaloshinskiĭ constant, $f(\frac{1}{2}M_1^2, \frac{1}{2}M_2^2)$ is the exchange energy, which determines the values of the magnetic moments at a given temperature, $\mathbf{M}_1$ and $\mathbf{M}_2$ are the sublattice magnetizations, and **n** is a unit vector along the symmetry axis; we shall henceforth need also the quantities

$$\mathbf{l} = \frac{1}{2}\left(\frac{\mathbf{M}_1}{M_1} - \frac{\mathbf{M}_2}{M_2}\right) \qquad \mathbf{m} = \frac{1}{2}\left(\frac{\mathbf{M}_1}{M_1} + \frac{\mathbf{M}_2}{M_2}\right).$$