a consideration of Eqs. (17) and (25) that the strongcoupling approximation is in better correspondence with the nature of the interaction of the type γ_5 than the weak-coupling approximation.

The model we have considered gives an idea of the behavior of the Green function of the nucleon in pseudoscalar meson theory in the region $k^2 \gg m^2$, *i.e.*, far from the pole $k^2 = m^2$. Feynman¹² calculated the polarization of the vacuum in the approximation $\varphi(x) = \text{const}$; on the basis of the study of our model it can be said that his conclusion about the large part played by the polarization of the vacuum relates only to the region $k^2 \gg m^2$.

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¹ V. G. Solov'ev, Dokl. Akad. Nauk SSSR 108, 1041 (1956).

²T. D. Lee, Phys. Rev. 95, 1329 (1954).

³G. Källen and W. Pauli, Kgl. Dansk. Mat. Fys. Medd. 30, No. 7 (1955). Y. Munakata, Prog. Theoret. Phys. 13, 455, (1955).

⁴ N. N. Bogoliubov and D. V. Shirokov, Dokl. Akad. Nauk SSSR 105, 685 (1955). ⁵ H. Umezawa and A. Visconti, Nuclear Physics 1, 20 (1956).

⁶ K. Tanaka, Phys. Rev. 99, 676 (1955).

⁷B. Bosko and R. Stroffolini, Nuovo cimento 2, 133 (1955); 3, 662 (1956).

⁸ S. Machida, Prog. Theoret. Phys. 14, 407 (1955).

⁹ W. Thirring, Helv. Phys. Acta 28, 344 (1955).

¹⁰ A. A. Abrikosov and I. M. Khalatnikov, Dokl. Akad. Nauk SSSR 103, 993 (1955).

¹¹N. N. Bogoliubov, Dokl. Akad. Nauk SSSR **99**, 225 (1954).

¹²R. Feynman, Proc. Fifth Rochester Conf. (1955).

¹³ E. T. Whittaker and G. N. Watson, A Course of Modern Analysis, Part I.

¹⁴G. Hardy, Divergent Series.

¹⁵ N. N. Bogoliubov and D. V. Shirkov, Prog. Phys. Sci. 55, 148; 57, 3 (1955).

¹⁶H. Lehmann, Nuovo cimento 11, 342, (1954).

¹⁷M. Gell-Mann and F. Low, Phys. Rev. 95, 1300 (1954).

¹⁸G. Källen, Kgl. Dansk. Mat. Fys. Medd. 27, No. 12 (1953); Helv. Phys. Acta 25, 417 (1952).

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Extension of the Spin-Wave Model to the Case of Several Electrons Surrounding Each Site

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The energy of a weakly excited state of a ferromagnetic or antiferromagnetic crystal in which each site is surrounded by several electrons is calculated by the method of approximate second quantization, applied to a system consisting of two types of interacting Fermi particles. It is found that besides the usual excitations of the ferromagnon-antiferromagnon type, some additional excitations, which depend weakly on the quasi-momentum, appear in these systems. A physical interpretation of these excitations is proposed.

1. THE PICTURE OF a weakly excited state of a ferromagnetic or antiferromagnetic crystal, when there is only one magnetically active electron at each lattice site, is now fairly well understood. In the approximations of the spin-wave model it is possible to approximate the energy of a weaklyexcited state of these crystals by the energy of an ideal gas of separate Bose-type quasi-particlesferromagnons¹ antiferromagnons^{2, 3, 4} obeying the dispersion laws

$$E_{\mu} = \frac{1}{2} c J (a\mu)^2, \quad E_{\mu} = \frac{1}{2} c J (a\mu)$$
 (1)

respectively for ferromagnets and antiferromagnets, whereupon two independent branches of excitations are obtained for antiferromagnets. Here μ is the quasi-momentum, J the exchange integral between nearest neighbors, and c the number of these nearest neighbors.

According to the model of Bloch¹, each of these quasi-particles corresponds to the motion of an inverted electron spin through the ordered array of the remaining spins. This simplified homeopolar model leads to qualitative results which agree with experiment. Real ferromagnetic or antiferromagnetic crystals, however, have several electrons with uncompensated spins at each site.

The first attempt to allow for the existence of several electrons per atom in a ferromagnetic crystal was made in a very approximate form by Möller⁵, who considered all the electrons of the atom to be in a single state. This approach was so crude that Möller was not able to obtain any new qualitative results.

Recently Kondorskii and Pakhomov⁶ have carried out a more accurate calculation of the energy of a ferromagnetic crystal with several electrons per atom. In this paper we will solve the analogous problem for antiferromagnetic crystals. Since the spectra of ferromagnets and antiferromagnets have a great many regularities in common, it is expedient to study them together within a single mathematical scheme. For this purpose we will consider a Hamiltonian of fairly general type which describes a system consisting of two types of interacting Fermi particles, and determine its lowest eigenvalues by the method of approximate second quantization of Bogoliubov and Tiablikov^{7, 8} which they developed for a system made up of identical particles.

By considering the electrons of the individual sublattices in an antiferromagnet as particles of different kinds, we can imagine the Hamiltonian of an antiferromagnet to be a special case of our general Hamiltonian; the Hamiltonian of a ferromagnet will be contained in it automatically. We will thus be able to solve the problem for ferromagnets and antiferromagnets at the same time.

2. We will consider a crystalline system at the nodes of which there are two different types of Fermi particles, but with only one particle at each node. In addition to the principal S-state of the isolated atom there will be other states with large degeneracy. Let us say that the wave function of these states will be $\varphi_{f\nu}(q, s)$, where ν runs through a finite set of values. We will suppose that the interatomic spacings are sufficiently large to guarantee that there will be little overlapping of the electronic orbits. In the representation of second quantization the Hamiltonian of such a system is written in the form:

$$\hat{H} = \sum A (f_1 v_1 v_1') a_{f_1 v_1}^+ a_{f_1 v_1'}^+ + \sum C(g_1 v_1 v_1') c_{g_1 v_1}^+ c_{g_1 v_1'}^+ + \frac{1}{2} \sum B (f_1 f_2 v_1 v_2 v_1' v_2') a_{f_1 v_1}^+ a_{f_2 v_2}^+ a_{f_2 v_2'}^+ a_{f_1 v_1'}^+ + \frac{1}{2} \sum' D (g_1 g_2 v_1 v_2 v_1' v_2') c_{g_1 v_1}^+ c_{g_2 v_2}^+ c_{g_2 v_2'}^- c_{g_1 v_1'}^+ + \sum E (f_1 g_2 v_1 v_2 v_1' v_2') a_{f_1 v_1}^+ a_{f_1 v_1'}^+ c_{g_2 v_2}^+ c_{g_2 v_2'}^-,$$
(2)

(each term is summed over all indices), in which

$$\sum_{\nu} a_{f\nu}^+ a_{f\nu} = 1, \quad \sum_{\nu} c_{g\nu}^+ c_{g\nu} = 1.$$
(3)

Here the indices f and g designate the sites at which the Fermi particles of respective types are located: $a_{f\nu}$ and $c_{g\nu}$ are self-commuting Fermioperators.

Following the basic idea of the method of approximate second quantization, we select two system functions $\theta_{\omega}(f\nu)$ and $\Phi_{\omega}(g\nu)$ such that

$$\sum_{\nu} \theta_{\omega}^{*} (f\nu) \theta_{\omega'} (f\nu) = \delta (\omega - \omega'),$$

$$\sum_{\nu} \Phi_{\omega}^{*} (g\nu) \Phi_{\omega'} (g\nu) = \delta (\omega - \omega')$$
(4)

(where ω takes the same values as ν) and require that $\theta_0(f\nu)$ and $\Phi_0(g\nu)$ yield a minimum for Eq. (2) under the condition (3), if the operators in these expressions are replaced by the usual *c*-numbers.

We now consider a canonical transformation

$$a_{f\nu} = \sum_{\omega} \theta_{\omega} (f\nu) a_{f\omega}, \quad c_{g\nu} = \sum_{\omega} \Phi_{\omega} (g\nu) c_{g\omega} \qquad (5)$$

of the Fermi operators $a_{f\nu}$ and $c_{f\nu}$ to new Fermi operators $a_{f\omega}$ and $c_{g\omega}$. We determine the functions $\theta_{\omega}(f\nu)$ and $\Phi_{\omega}(g\nu)$ for $\omega \neq 0$ by requiring that they obey the equations:

$$\begin{split} \sum_{\mathbf{v}_{1}'} A \left(f_{1} \mathbf{v}_{1} \mathbf{v}_{1}'\right) \theta_{\omega} \left(f_{1} \mathbf{v}_{1}'\right) &+ \sum_{f_{2}(\neq f_{1}) \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'} B \left(f_{1} f_{2} \mathbf{v}_{1} \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'\right) \theta^{*} \left(f_{2} \mathbf{v}_{2}\right) \theta \left(f_{2} \mathbf{v}_{2}'\right) \theta_{\omega} \left(f_{1} \mathbf{v}_{1}'\right) \\ &+ \sum_{g_{2} \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'} E \left(f_{1} g_{2} \mathbf{v}_{1} \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'\right) \theta_{\omega} \left(f_{1} \mathbf{v}_{1}'\right) \Phi^{*} \left(g_{2} \mathbf{v}_{2}\right) \Phi \left(g_{2} \mathbf{v}_{2}'\right) \\ &= \lambda_{\omega} \left(f_{1}\right) \theta_{\omega} \left(f_{1} \mathbf{v}_{1}\right). \end{split}$$
(6)
$$\sum_{\mathbf{v}_{2}'} C \left(g_{2} \mathbf{v}_{2} \mathbf{v}_{2}'\right) \Phi_{\omega} \left(g_{2} \mathbf{v}_{2}'\right) + \sum_{g_{1}(\neq g_{2}) \mathbf{v}_{1} \mathbf{v}_{2}' \mathbf{v}_{1}'} D \left(g_{1} g_{2} \mathbf{v}_{1} \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'\right) \Phi_{\omega} \left(g_{2} \mathbf{v}_{2}'\right) \Phi \left(g_{1} \mathbf{v}_{1}'\right) \\ &\times \Phi^{*} \left(g_{1} \mathbf{v}_{1}\right) + \sum_{f_{1} \mathbf{v}_{1} \mathbf{v}_{1}' \mathbf{v}_{2}'} E \left(f_{1} g_{2} \mathbf{v}_{1} \mathbf{v}_{2} \mathbf{v}_{1}' \mathbf{v}_{2}'\right) \theta^{*} \left(f_{1} \mathbf{v}_{1}\right) \theta \left(f_{1} \mathbf{v}_{1}'\right) \Phi_{\omega} \left(g_{2} \mathbf{v}_{2}'\right) \\ &= \lambda_{\omega} (g_{2}) \Phi_{\omega} (g_{2} \mathbf{v}_{2}), \end{split}$$

multipliers.

These equations make it possible for us to eliminate from the Hamiltonian, expressed in the new Fermi operators, those terms which contain only one non-zero index ω . Retaining first-order terms (those with two non-zero indices ω) in the Hamiltonian, we find that we can introduce new operators constructed from Fermi operators in the following way:

$$b_{f\omega} = a_{f_0}^+ a_{f\omega}, \ d_{g\omega} = c_{g_0}^+ c_{g\omega},$$

$$b_{f\omega}^+ = a_{f\omega}^+ a_{f_0}, \ d_{g\omega}^+ = c_{g\omega}^+ c_{g_0}.$$
(7)

As it turns out, the operators (7) satisfy Bose commutation relations approximately if we consider

where $\lambda_{\omega}(f\nu)$ and $\lambda_{\omega}(g\nu)$ are undetermined Lagrangian the weak interactions of the system. It is easy to show that the original Hamiltonian (2) is represented in this approximation by a quadratic form in the Bose operators $b_{g\omega}$ and $d_{f\omega}$.

> The diagonalization of the quadratic form obtained above can be carried out by the usual methods.^{7,8} For the energy of the system which we are studying we obtain:

$$E = E_0 + \sum_j \sum_{\mu} E^j_{\mu} n^j_{\mu}, \quad n^j_{\mu} = 0, 1, 2, \dots, (8)$$

where E^{j}_{μ} is determined from the characteristic equation of the system of homogeneous linear equations:

$$\Phi^{-}(f\omega) c_{1\mu}(\omega) + \sum_{\omega_{2}} \{q(f\omega\omega_{2}) c_{1\mu}(\omega_{2}) + p(f\omega\omega_{2}) c_{2\mu}(\omega_{2}) + k^{*}(f\omega\omega_{2}) c_{3\mu}(\omega_{2}) + t(f\omega\omega_{2}) c_{4\mu}(\omega_{2})\} = 0.$$

$$\Phi^{+}(f\omega) c_{2\mu}(\omega) + \sum_{\omega_{2}} \{p(f\omega\omega_{2}) c_{1\mu}(\omega_{2}) + q^{*}(f\omega\omega_{2}) c_{2\mu}(\omega_{2}) + t^{*}(f\omega\omega_{2}) c_{3\mu}(\omega_{2}) + k(f\omega\omega_{2}) c_{4\mu}(\omega_{2})\} = 0.$$

$$\Phi^{-}(g\omega) c_{3\mu}(\omega) + \sum_{\omega_{2}} \{k(g\omega_{2}\omega) c_{1\mu}(\omega_{2}) + t(g\omega_{2}\omega) c_{2\mu}(\omega_{2}) + q(g\omega\omega_{2}) c_{3\mu}(\omega_{2}) + p(g\omega\omega_{2}) c_{4\mu}(\omega_{2})\} = 0.$$

$$\Phi^{+}(g\omega) c_{4\mu}(\omega) + \sum_{\omega_{2}} \{t^{*}(g\omega_{2}\omega) c_{1\mu}(\omega_{2}) + k(g\omega_{2}\omega) c_{2\mu}(\omega_{2}) + p(g\omega\omega_{2}) c_{3\mu}(\omega_{2}) + q^{*}(g\omega\omega_{2}) c_{4\mu}(\omega_{2})\} = 0,$$
(9)

in which the following matrices have been introduced

$$q (f\omega_{1} \omega_{2}) = \sum_{f_{2}}' e^{i\mu(f_{2}-f)} \sum_{\nu_{1}\nu_{2}\nu_{1}'\nu_{2}'} B (ff_{2}\nu_{1}\nu_{2}\nu_{1}'\nu_{2}') \theta_{\omega_{1}}^{*} (f\nu_{1}) \theta^{*} (f_{2}\nu_{2}) \theta_{\omega_{2}} (f_{2}\nu_{2}') \theta (f\nu_{1}').$$

$$p (f\omega_{1}\omega_{2}) = \sum_{f_{2}} e^{i\mu(f_{2}-f)} \sum_{\nu_{1}\nu_{2}\nu_{1}'\nu_{2}'} B (ff_{2}\nu_{1}\nu_{2}\nu_{1}'\nu_{2}') \theta_{\omega_{1}}^{*} (f\nu_{1}) \theta_{\omega_{2}}^{*} (f_{2}\nu_{2}) \theta (f_{2}\nu_{2}') \theta (f\nu_{1}').$$

$$k (f\omega_{1}\omega_{2}) = \sum_{g_{2}}' e^{i\mu(g_{2}-f)} \sum_{\nu_{1}\nu_{2}\nu_{1}'\nu_{2}'} E (fg_{2}\nu_{1}\nu_{2}\nu_{1}'\nu_{2}') \theta_{\omega_{1}}^{*} (f\nu_{1}) \theta (f\nu_{1}') \Phi_{\omega_{2}}^{*} (g_{2}\nu_{2}) \Phi (g_{2}\nu_{2}').$$

$$t (f\omega_{1}\omega_{2}) = \sum_{g_{2}} e^{i\mu(g_{2}-f)} \sum_{\nu_{1}\nu_{2}\nu_{1}'\nu_{2}'} E (fg_{2}\nu_{1}\nu_{2}\nu_{1}'\nu_{2}') \theta^{*} (f\nu_{1}) \theta_{\omega_{2}} (f\nu_{1}') \Phi_{\omega_{1}}^{*} (g_{2}\nu_{2}) \Phi (g_{2}\nu_{2}').$$

$$\Phi^{\mp} (f\omega) = \lambda_{\omega} (f) - \lambda_{0} (f) \mp E_{\mu}.$$
(10)

3. We now allow for the existence of several electrons per site and look into the two possibilities.

1. Ferromagnetism. According to Bogoliubov⁸, the Hamiltonian of a ferromagnetic crystal with allowance for the electronic excited states is written in the form:

$$\dot{H} = U_0$$

$$\frac{1}{2} \sum_{f_1 \lambda_1 \neq f_2 \lambda_2 \sigma_1 \sigma_2} J\left(f_1 \lambda_1 f_2 \lambda_2\right) a_{f_1 \lambda_1 \sigma_1}^+ a_{f_2 \lambda_2 \sigma_2}^+ a_{f_2 \lambda_2 \sigma_1} a_{f_1 \lambda_1 \sigma_2}$$

$$(11)$$

together with the conditions of homeopolarity

$$\sum_{\sigma} a_{f\lambda\sigma}^+ a_{f\lambda\sigma} = 1, \qquad (12)$$

according to which there is at the node f only one electron in the state λ ; $\lambda = 1, 2 \dots z$, where z is the number of occupied states (the number of electrons per site).

For a positive exchange integral $J(f_1\lambda_1f_2\lambda_2) > 0$ the solution of the system of equations (6) can be put in the form

$$\begin{split} \theta_{\omega}\left(f\lambda\nu\right) &= \delta\left(\nu - \omega\right), \quad \Phi_{\omega}\left(g\lambda\nu\right) \equiv 0, \\ \nu &= \sigma + \frac{1}{2} = 0; 1. \end{split}$$

It is easy to show that in this case the basic equations (10) agree with the equations of Kondorskii and Pak homov⁶.

By applying the method of "perturbations" to the equations obtained above we can find that for small values of the quasi-momentum μ the solution of the system has the following structure:

$$E_{\mu}^{i} = (c/2z) (a\mu)^{2} \sum_{ij} J_{ij},$$

$$E_{\mu}^{2} = E_{\mu2}^{(0)} + E_{\mu2}^{(1)} (a\mu)^{2}, \dots \qquad (13)$$

$$E_{\mu}^{z} = E_{\mu z}^{(0)} + E_{\mu z}^{(1)} (a\mu)^{2},$$

where the last z - 1 quantities are determined by the mutual relations between the exchange integrals. If it is assumed that the exchange integrals between different states are $J_{ij} = J$; $J_{ij}^0 = J^0$, which seems to be approximately true for real crystals, then the solutions of (13) are

$$E^{1}_{\mu} = \frac{1}{2} czJ (a\mu)^{2}, \quad E^{k}_{\mu} = z (J^{0} + cJ),$$

 $k = 2, 3, \ldots, z.$
(14)

Comparing Eqs. (13) and (14) we see that in a ferromagnet only one of the z branches of the spectrum depends quadratically on the quasi-momentum. For the other z - 1 branches the large constant term overlaps the small one which depends on the quasimomentum and which all but disappears if the exchange integrals differ little for different states.

2. Antiferromagnetism. We take for the Hamiltonian of an antiferromagnet

$$\hat{H} = E_{0}$$

$$-\frac{1}{2} \sum_{f_{1}\lambda_{1}g_{2}\lambda_{2}\sigma_{1}\sigma_{2}} J \left(f_{1}\lambda_{1}g_{2}\lambda_{2}\right) a_{f_{1}\lambda_{1}\sigma_{1}}^{+} a_{f_{1}\lambda_{1}\sigma_{2}} c_{g_{2}\lambda_{2}\sigma_{2}}^{+} c_{g_{2}\lambda_{2}\sigma_{1}}$$
(15)

with the conditions

$$\sum_{\sigma} a_{f\lambda\sigma}^+ a_{f\lambda\sigma} = 1; \quad \sum_{\sigma} c_{g\lambda\sigma}^+ c_{g\lambda\sigma} = 1.$$

Now the solution of the system of equations (6) will be

$$\theta_{\omega}(f\lambda v) = \delta(v - \omega), \quad \Phi_{\omega}(g\lambda v) = \delta(v + \omega - 1).$$

Under these conditions, after approximations analogous to those made for a ferromagnet, the secular equation of the system of equations (9) has 2z positive solutions:

$$\begin{split} E^{1}_{\mu} &= \frac{1}{2} \, z c J \, (a \mu), & \text{multiplicity } 2 \\ E^{i}_{\mu} &= z \, (J^{0} + c J \, / \, 2), & \text{multiplicity } 2(z-1). \end{split}$$

Thus it is found that when there are z electrons per atom a ferromagnet has z independent branches of Bose-type excitations, while an antiferromagnet has 2z branches.

In addition to the usual excitations of ferromagnonantiferromagnon type some new excitations arise, which depend weakly on the quasi-momentum and vanish for z = 1.

4. In order to explain the physical meaning of

these special excitations which depend weakly on
the quasi-momentum, we consider still another sub-
sidiary problem: let us find the energy of a weakly
excited state of a ferromagnetic crystal with one
electron per site, in which, in addition to the
S-state, there are other excited states, designated
by the index
$$\lambda$$
, which arbitrarily assume the values
 $0, 1, \dots (z - 1)$. In all there will be $2z$ different
electronic states per atom, since for each "orbit"
the electron can have two spin directions. If it is
assumed that an electron with a given spin direc-
tion is in its ground state, then all told there will
be $2z - 1$ different excited states possible for the
electrons inside each atom.

From Bogoliubov's general scheme⁸ it is a simple matter to obtain an expression for the Hamiltonian of this system. If we require that the following condition be satisfied:

$$\sum_{\lambda\sigma} a_{f\lambda\sigma}^+ a_{f\lambda\sigma} = 1, \qquad (16)$$

then the Hamiltonian takes the form

$$\hat{H} = \sum_{f\lambda\lambda'\sigma} L\left(f\lambda f\lambda'\right) a_{f\lambda\sigma}^{+} a_{f\lambda'\sigma} + \frac{1}{2} \sum_{(f\lambda)\sigma_{1}\sigma_{2}} F\left(f_{1}\lambda_{1}f_{2}\lambda_{2}f_{1}\lambda'_{1}f_{2}\lambda'_{2}\right) a_{f_{1}\lambda_{1}\sigma_{2}}^{+} a_{f_{2}\lambda_{2}\sigma_{1}}^{+} \\ \times a_{f_{2}\lambda'_{2}\sigma_{2}} a_{f_{1}\lambda'_{1}\sigma_{1}} - \frac{1}{2} \sum_{(f\lambda)\sigma_{1}\sigma_{2}} F\left(f_{1}\lambda_{1}f_{2}\lambda_{2}f_{2}\lambda'_{2}f_{1}\lambda'_{1}\right) a_{f_{1}\lambda_{1}\sigma_{1}}^{+} a_{f_{2}\lambda_{2}\sigma_{2}}^{+} a_{f_{2}\lambda'_{2}\sigma_{1}}^{+} a_{f_{1}\lambda'_{1}\sigma_{2}}^{+}.$$
(17)

Now let us renormalize the quantity σ and assume that it takes the values 0, 1: this change will not affect our results. Since $\nu = (\lambda \sigma)$, then $\omega = (\Lambda \Sigma)$. If we take the functions

$$\theta_{\Lambda\Sigma}(f\lambda\sigma) = \delta(\lambda - \Lambda) \,\delta(\sigma - \Sigma), \quad \Phi_{\Lambda\Sigma}(g\lambda\sigma) \equiv 0,$$

as solutions of Eq. (6), it is not difficult to show that the non-zero coefficients in Eq. (10) will be

$$p_{\mu} (f \Lambda 0 \Lambda_{2} 0) = \sum_{f_{2}(\neq f)} e^{i\mu(f_{2}-f)} \operatorname{Re} [F (f \Lambda f_{2} \Lambda_{2} f 0 f_{2} 0) - F (f \Lambda f_{2} \Lambda_{2} f_{2} 0 f 0)],$$

$$q_{\mu} (f \Lambda 0 \Lambda_{2} 0) = \sum_{f_{2}(\neq f)} e^{i\mu(f_{2}-f)} [F (f \Lambda f_{2} 0 f 0 f_{2} \Lambda_{2}) - F (f \Lambda f_{2} 0 f_{2} \Lambda_{2} f 0)],$$

$$q_{\mu} (f \Lambda 1 \Lambda_{2} 1) = -\sum_{f_{2}(\neq f)} e^{i\mu(f_{2}-f)} F (f \Lambda f_{2} 0 f_{2} \Lambda_{2} f 0).$$
(18)

For the problem at hand the characteristic equation of the system (9) breaks up into three equations:

$$\det \| q_{\mu} (f\Lambda 1 \Lambda_{2} 1) + \Phi^{-} (f\Lambda 1) \delta_{\Lambda\Lambda_{2}} \| \cdot \det \| q_{\mu}^{*} (f\Lambda 1 \Lambda_{2} 1) + \Phi^{+} (f\Lambda 1) \delta_{\Lambda\Lambda_{2}} \| = 0,$$

$$\det \left\| \frac{q_{\mu} (f\Lambda 0\Lambda_{2} 0) + \Phi^{-} (f\Lambda 0) \delta_{\Lambda\Lambda_{2}}}{p_{\mu} (f\Lambda 0\Lambda_{2} 0)} \right\| \frac{p_{\mu} (f\Lambda 0\Lambda_{2} 0)}{q_{\mu}^{*} (f\Lambda 0\Lambda_{2} 0) + \Phi^{+} (f\Lambda 0) \delta_{\Lambda\Lambda_{2}}} \right\| = 0.$$
(19)

The first two equations in (19) are each of order z; the third, of order 2z - 1. It is not difficult to show that if E_{μ} is a root of Eq. (19), then $-E_{\mu}$ will also be a root, so that there will be 2z - 1 positive solutions.

In the determinants of the matrices on the left hand side of Eq. (19) there appear only matrix elements with $\Sigma = 0$ or with $\Sigma = 1$; consequently we conclude that the group of eigenvalues of the Hamiltonian (17) can be split up into two independent subgroups—one with spin excitations, one without. The equations of order z describe the spin excitations of the crystal. For the case z = 2 they are easily solved and yield two positive solutions:

$$E_{\mu}^{-} = \frac{1}{2} \Delta_{10} + 2cJ_{10} + \frac{1}{4} (J_{00} + J_{11} - 2J_{10}) c (a\mu)^2,$$

$$E_{\mu}^{+} = \frac{1}{2} \Delta_{10} + \frac{1}{4} (J_{00} + J_{11} + 2J_{10}) c (a\mu)^2, \quad (20)$$

where $J_{\Lambda_1\Lambda_2} = F(f\Lambda_1f_20f_2\Lambda_2f_0)$ are the exchange in-

tegrals between two electrons Λ_1 and Λ_2 of neighboring atoms, occupying either the ground state or excited states. Δ_{10} is just the difference between the levels of the electrons in an atom of the crystal.

We now turn our attention to a deep analogy which exists between Eqs. (20) and the equations of Kondorskii and Pakhomov⁶. The latter describe the spin excitations which arise out of nearest-neighbor interactions of atoms, each of which has two electrons fixed in their "orbits." Equations (20), however, describe the analogous excitations for a system in which each atom has one electron in the lower state, so that in order to transfer the electron to the next "orbit" it is necessary to supply it with an energy Δ_{10} . Consequently Eqs. (20) describe the spin excitations after part of the electrons has already gone into the excited state. We will not investigate the excitations without spin here.

We have carried out an analysis of the solution for z = 2. Great technical difficulties arise for the other cases. We assume that the exchange integrals J_{ii} are identical for different pairs of states (*ji*).

In this case the first equation of (19) yields

$$E^{i}_{\mu} = f(\Delta_{ij}) + czJ, \ (z-1); \ E^{1}_{\mu} = A(a\mu)^{2}, \ (21)$$

where $f(\Delta_{ij})$ is some function of Δ_{ij} , the difference between energy levels, which vanishes when $\Delta_{ij} = 0$. Equation (20) now becomes identical with Eq. (14) for a ferromagnet with z electrons per atom. Thus we come to the conclusion that in a system with several electrons per atom, the appearance of the new excitations which depend weakly on the quasi-momentum is connected with the possibility of exchange between electrons separated by energy gaps.

We still have to explain the significance of the solutions which depend on the quasi-momentum:

$$E^{1}_{\mu} = \frac{1}{2} cz J (a\mu)^{2}.$$
 (22)

In the ground state at each site there are up to z electrons with their spins directed, say, to the left. The total spin at this node will be -z/2. If at a site there were just one particle with spin s = z/2, instead of z electrons with spins s = 1/2, the number of possible orientations of this spin would be 2s + 1 = z + 1. Such particles could have z excited states. The solution of the problem for these particles would be

$$E^{j}_{\mu} = \frac{1}{2} cJ (a\mu)^{2}, \quad j = 1, 2, \ldots z.$$

If we compare this expression with the first equation of (1), we come to the conclusion that each such excitation has to correspond to a change of the spin projection by unity. Then a change of the spin projection by z units has to correspond to the energy

$$E_{\mu} = \frac{1}{2} zc J (a\mu)^2, \qquad (23)$$

whereupon the spin projection becomes equal to z/2, *i.e.*, the spin flips over. But Eq. (23) agrees with (22), so that latter ought to correspond to a change of the spin projection by z units, *i.e.*, the entire group of spins surrounding the atom flips over as a whole. We did not find any other excitations of the system which depend on the quasimomentum in the same way, so we conclude that in a ferromagnetic crystal (containing up to z magnetically active electrons per atom) spin waves are propagated in which a whole group of spins at the site acts as a unit. This is a natural extension of the idea of a ferromagnon to the case of z electrons surrounding the site.

For antiferromagnets the interpretation of the elementary excitations has to be analogous.

In conclusion I take the opportunity to express sincere appreciation to Professor S. V. Vonsovskii and to G. G. Taluts for valuable discussions.

- ¹ F. Bloch, Z. Physik 74, 295 (1932).
- ² P. W. Anderson, Phys. Rev. 86, 694 (1952).
- ³ R. Kubo, Phys. Rev. 87, 568 (1952).
- ⁴ J. Tessman, Phys. Rev. 88, 1132 (1952).
- ⁵C. Möller, Z. Physik 82, 559 (1933).

⁶ E. Kondorskii and A. Pakhomov, Dokl. Akad. Nauk SSSR 93, 431 (1953). ⁷ N. N. Bogoliubov and S. V. Tiablikov, J. Exptl.
Theoret. Phys. (U.S.S.R.) 19, 256 (1949).
⁸ N. N. Bogoliubov, Lectures in Quantum Statistics, 1949.

⁹S. V. Tiablikov, Fiz. Metallov i Metallovedenie 2, 193 (1956).

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Equations with Variational Derivatives in Statistical Equilibrium Theory

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Equations with variational derivatives for correlation functions have been derived. A method is developed for solving these for various systems in statistical equilibrium. A "superposition" theorem is derived for obtaining the correlation functions when the interaction between the particles of the system can be described as the sum of long and short range forces.

T HE BEHAVIOR OF A statistical system of interacting particles is determined by the corresponding distribution functions of these particles $F_s(x_1, x_2, \ldots, x_s)$ $(s = 1, 2, 3, \ldots)$. Bogoliubov¹ has shown that the functions F_s can be represented by variational derivatives of the functional introduced by him, and the series of equations for the determination of these distribution functions were first obtained by him. As Bogoliubov also pointed out², his functional does not have a direct physical interpretation; he therefore pointed out a method in Ref. 2 for the construction of other functionals, based on the idea of the inclusion of the external field, in a manner similar to that employed in the Schwinger theory of the Green function.

In the present work, starting out from a functional for the free energy of a system of M types of particles in an external field $\varphi(x)$, closed equations are found with variational derivatives for the unitary distribution function for different forms of the functional argument; with the help of these derivatives, a method of determining the correlation functions has been deduced for systems of particles with different interactions: Coulombic $\Phi_0(r)$, an interaction decreasing rapidly with distance, $\Phi_1(r)$, and an interaction of the form $\Phi(r) = \Phi_0(r) + \Phi_1(r)$.

1. FREE ENERGY AS A FUNCTIONAL. DISTRIBUTION FUNCTIONS. EQUATIONS WITH VARIATIONAL DERIVATIVES

Let us consider a system of M types N_a molecules of the *a*th type. Let this system be located in an external field $\varphi(\mathbf{r})$. The probability density function of the position of the molecules is determined by the Gibbs function:

$$D = \frac{1}{Q} \exp\left\{-\frac{1}{\Theta} \left(U_N + \sum_{a,i} \varphi_a\left(\mathbf{r}_i\right)\right)\right\},$$

$$Q = \int \exp\left\{-\frac{1}{\Theta} \left(U_N + \sum_{a,i} \varphi_a\left(\mathbf{r}_i\right)\right)\right\} d\tau,$$

$$U_N = \sum \Phi_{ab}\left(|\mathbf{r}_{ai} - \mathbf{r}_{bj}|\right),$$
(1)

where U_N is the potential energy of interaction of the particles with each other; \mathbf{r}_{ai} determines the position of the *i*th molecule of the *a*th type, while the summation is taken over all different pairs of