

# Antiferromagnet in a strong magnetic field: analogy with Bose gas

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An antiferromagnet in a near-critical magnetic field can be regarded as an low-density assembly of Bose particles, so that the well-developed gas approximation can be used. This is demonstrated with spin-1/2 as the example. In the simplest cases it is easy to obtain an expression for the particle-scattering amplitude in terms of the initial exchange interaction, after which the known results for the Bose gas can yield the ground-state energy and other characteristics. The periods and the type of the spin structure are also determined. The dependence of the transition temperature on the magnetic field is found to be given by  $T_c \sim (H_c - H)^{2/3}$ .

## I. INTRODUCTION

The following approach is used in theory of antiferromagnets to determine the ground state.<sup>1</sup> In the zeroth approximation the spins are regarded as classical vectors and the corresponding expression for the energy is minimized. This procedure leads to a state with several sublattices having different spin directions. Excited states are considered in the next approximation; both the magnon spectrum and the correction to the energy to account for quantum fluctuations are obtained. This correction is usually small, thus attesting to the applicability of this scheme. In a magnetic field, the sublattice picture is preserved up to a critical field  $H_c$ , above which all the spins are aligned parallel; the calculation method remains accordingly likewise unchanged.

Near  $H_c$ , however, another more consistent approach to the problem is possible, using the analogy with a Bose gas. The present paper is devoted to this question. Although the main idea was described by us earlier,<sup>2</sup> it makes sense to repeat it here.

First, the model. We confine ourselves to spin 1/2. Consider a system with a Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{n \neq n'} I_{nn'} \mathbf{S}_n \mathbf{S}_{n'} + H \sum_n S_{nz}, \quad (1)$$

where  $\mathbf{S}_n$  is the spin operator of site  $n$  and  $H$  is the magnetic field in energy units. We transform to Pauli operators:

$$S_{nz} = \beta_n^+ \beta_n^- - \frac{1}{2}, \quad S_n^+ = \beta_n^+, \quad S_n^- = \beta_n^-, \quad S_n^\pm = S_{nx} \pm i S_{ny}. \quad (2)$$

These operators commute at different sites, and on the same site they satisfy the relations

$$\beta_n \beta_n^+ + \beta_n^+ \beta_n^- = 1, \quad \beta_n^2 = (\beta_n^+)^2 = 0. \quad (3)$$

Having transformed to Pauli operators, we can refer to particles instead of spins, and this we shall do.

Substitution of (2) in (1) gives

$$\mathcal{H} = \mathcal{E}_0(H) + \mathcal{H}_0 + \mathcal{H}_1,$$

$$\mathcal{E}_0(H) = \frac{1}{4} \cdot \frac{1}{2} \sum_{n \neq n'} I_{nn'} - \frac{1}{2} H N,$$

$$\begin{aligned} \mathcal{H}_0 &= \frac{1}{2} \sum_{n \neq n'} I_{nn'} \beta_n^+ \beta_{n'}^- + \sum_n \left( H - \frac{1}{2} \sum_{n'} I_{nn'} \right) \beta_n^+ \beta_n^-, \\ \mathcal{H}_1 &= \frac{1}{2} \sum_{n \neq n'} I_{nn'} \beta_n^+ \beta_{n'}^+ \beta_{n'}^- \beta_n^-, \end{aligned} \quad (4)$$

where  $N$  is the number of sites in the lattice. We have grouped here the various contributions to the Hamiltonian. The energy  $\mathcal{E}_0(H)$  of the state with maximum spin (magnetic moment in terms of the spin) does not depend on the operators  $\beta$  and  $\beta^+$ ; we can use this quantity to write down the antiferromagnetism condition:

$$\mathcal{E}_0(0) > 0. \quad (5)$$

In Eq. (4),  $\mathcal{H}_0$  is the Hamiltonian component quadratic in the operators; the first term gives the band energy of a single particle. This energy can be found in the usual manner: the eigenfunctions  $\psi_p$  and the eigenenergy  $\varepsilon(p)$  of the single-particle problem are:

$$\begin{aligned} \psi_p &= \beta_p^+ |0\rangle, \quad \beta_p^+ = \frac{1}{N^{1/2}} \sum_n e^{ip\mathbf{R}_n} \beta_n^+, \\ \varepsilon(p) &= \frac{1}{2} \sum_{n'} I_{nn'} \exp\{ip(\mathbf{R}_{n'} - \mathbf{R}_n)\}, \end{aligned} \quad (6)$$

where  $\mathbf{p}$  is the quasimomentum,  $\mathbf{R}_n$  is the radius vector of site  $n$ , and summation over  $n' \neq n$  is implied in the last sum (and in all similar sums).

The second term of  $\mathcal{H}_0$  adds to the particle energy a quasi-momentum-independent contribution  $\bar{\varepsilon}$  which we express in the form

$$\bar{\varepsilon} = -\varepsilon_0 + (H - H_c), \quad \varepsilon_0 = \min \varepsilon(p), \quad (7)$$

where  $\varepsilon_0$  is the minimum value of  $\varepsilon(p)$ ; we have introduced here the critical magnetic field  $H_c$ :

$$H_c = \frac{1}{2} \sum_{n'} I_{nn'} - \varepsilon_0 \quad (8)$$

(the meaning of this definition will be made clear presently). We note that  $\varepsilon_0 < 0$  for an antiferromagnet; this follows from condition (5) and from the obvious identity

$$\langle \varepsilon \rangle = \frac{1}{N} \sum_p \varepsilon(p) = 0 \quad (9)$$

(the summation is over  $\mathbf{p}$ , as usual, is within the limits of the Brillouin cell). The energy  $\omega(\mathbf{p})$  of a single particle with quasimomentum  $\mathbf{p}$  is thus the sum of (6) and (7), i.e.,

$$\omega(\mathbf{p}) = [\varepsilon(\mathbf{p}) - \varepsilon_0] + (H - H_c). \quad (10)$$

Finally,  $\mathcal{H}_1$  is the particle interaction; this operator determined jointly with conditions (3) the number of particles at  $H < H_c$ .

We proceed now to an exposition of the main basic idea of the paper. In a field  $H > H_c$  all the spins are parallel; the elementary excitation of such a state is a ferromagnetic magnon with energy  $\omega(\mathbf{p})$  [Eq. (10)]. Its energy is positive and its state stable so long as  $H > H_c$  [this clears up the meaning of the definition (8)]. We consider now  $H < H_c$ ; the state with parallel spins becomes unstable, since accumulation of negative energies is energywise favored [near the minimum of  $\omega(\mathbf{p})$ ]. Of course, the number of particles at  $H_c - H \ll H_c$  is small, i.e., we have a gas and we can use the gas approximation for the solution.

The gas approximation was developed for both Fermi and Bose particles. In our case there are neither, so that a reformulation of the problem is necessary.

Flipped spins cannot be regarded as Bose particles because of condition (3), which excludes centers occupied by two (and more) particles. This hindrance, however, can be taken into account differently by introducing infinite repulsion at the center:

$$\mathcal{H}' = U \sum_n \beta_n^+ \beta_n^+ \beta_n \beta_n, \quad U \rightarrow \infty, \quad (11)$$

after which restriction (3) can be lifted and  $\beta$  and  $\beta^+$  regarded as Bose operators.

We add thus to the Hamiltonian (4) the interaction (11) and obtain the initial Hamiltonian of our problem, but now for Bose particles. Transforming to quasimomenta [see Eq. (6)] we have

$$\mathcal{H} \rightarrow \sum_{\mathbf{p}} \omega(\mathbf{p}) \beta_{\mathbf{p}}^+ \beta_{\mathbf{p}} + \frac{1}{N} \sum_{\mathbf{p}_1} [U + \varepsilon(\mathbf{p}_1 - \mathbf{p}_2)] \beta_{\mathbf{p}_1}^+ \beta_{\mathbf{p}_2}^+ \beta_{\mathbf{p}_3} \beta_{\mathbf{p}_4}. \quad (12)$$

We have left out of  $\mathcal{H}$  the inessential constant  $\mathcal{C}_0(H)$ , and the usual quasimomentum conservation law is implied in the second sum.

Close to  $H_c$ , an antiferromagnet can thus be regarded as a weakly ideal Bose gas, so that the known results of Refs. 3 and 4 can be used.

We emphasize that we are forgoing the use of the sublattice state as the starting point. It is clear from the preceding that the particle concept and the analogy with a gas are more natural. What this leads to will be shown in Sec. 3. In the next section we discuss briefly certain problems not considered in the preceding ones.

## 2. GROUND STATE, EXCITATION SPECTRUM

The fullest analogy with the usual Bose gas takes place in the case of one minimum of  $\varepsilon(\mathbf{p})$  in the band; we confine ourselves to this case.

A single minimum must be located at the boundary of

the Brillouin zone at equivalent points that differ from one another by the reciprocal-lattice vector. It suffices therefore to introduce the coordinate  $\mathbf{p}_0$  of one of these points

$$\varepsilon(\mathbf{p}_0) = \varepsilon_0 = \min \varepsilon(\mathbf{p}).$$

By analogy with a Bose gas, the ground state of the system considered is a state with a Bose-Einstein condensate.<sup>3-4</sup> Of course, the particles accumulate to form a condensate at the minimum of the band, i.e., at  $\mathbf{p} = \mathbf{p}_0$ , and not with zero momentum as in the usual Bose gas (this difference is of no importance).

An important role is played in a gas by pair collisions, so that to determine the ground-state energy and other characteristics it suffices, in the lowest-order approximations in density, to find only one solitary constant—the scattering amplitude of two particles with energy at the minimum of the band and without taking the other particles into account. The latter means that the corresponding vertex part  $\Gamma$  is calculated with the aid of zeroth Green's functions, i.e., we have for it the so-called “ladder”

$$(13)$$

The summary frequency of the function  $\Gamma$  is chosen in accordance with the foregoing. We are interested in the value of  $\Gamma(\mathbf{p}_0)$ . The analytic form of Eq. (13) is

$$\Gamma(\mathbf{p}) = U + \varepsilon(\mathbf{p} - \mathbf{p}_0) - \frac{1}{N} \sum_{\mathbf{k}} \frac{U + \varepsilon(\mathbf{p} - \mathbf{k})}{\varepsilon(\mathbf{k}) - \varepsilon_0} \Gamma(\mathbf{k}) \quad (14)$$

(integration was carried out here with respect to the inner frequency).

In the limit as  $U \rightarrow \infty$  it is convenient to transform to a different function:

$$\Gamma(\mathbf{p}) = \Gamma_0 + \Gamma_1(\mathbf{p}),$$

$$\Gamma_0 = \frac{U}{1 + U\tau} \Big|_{U \rightarrow \infty} = \frac{1}{\tau}, \quad \tau = \left\langle \frac{1}{\varepsilon - \varepsilon_0} \right\rangle. \quad (15)$$

The operation  $\langle \dots \rangle$  is defined by Eq. (9);  $\Gamma_0$  is the vertex part for the XY model. As a result we get in lieu of (14)

$$\begin{aligned} \Gamma_1(\mathbf{p}) &= \langle \Gamma_1 \rangle + \varepsilon(\mathbf{p} - \mathbf{p}_0) - \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{p} - \mathbf{k})}{\varepsilon(\mathbf{k}) - \varepsilon_0} [\Gamma_0 + \Gamma_1(\mathbf{k})], \\ \left\langle \frac{\Gamma_1}{\varepsilon - \varepsilon_0} \right\rangle &= 0. \end{aligned} \quad (16)$$

These equations define  $\Gamma_1(\mathbf{p})$  and  $\langle \Gamma_1 \rangle$ .

Solution of this system entails in the simplest cases no difficulty. In actual calculations and estimates we shall have in mind mainly a simple cubic (SC) lattice with nearest-neighbor interaction. For this lattice,

$$\varepsilon(\mathbf{p}) = I(\cos p_x + \cos p_y + \cos p_z), \quad \mathbf{p}_0 = \pi(1, 1, 1), \quad m = 1/I, \quad (17)$$

where  $I > 0$  is the interaction between the nearest neighbors, the distance between which is taken to be unity; the coordinates of the band minimum and the effective mass  $m$  at the

minimum are also given.

We seek the solution of (16) in the form

$$\Gamma_i(\mathbf{p}) - \langle \Gamma_i \rangle \sim \varepsilon(\mathbf{p}).$$

As a result we get

$$\Gamma_i(\mathbf{p}) = \frac{1-\tau[\varepsilon(\mathbf{p})-\varepsilon_0]}{\tau(vI\tau-1)}, \quad \varepsilon_0 = -\frac{vI}{2}, \quad (18)$$

where  $v$  is the number of nearest neighbors (in this form, the solution is valid also for a *bcc* lattice). Adding Eq. (18) at the point  $\mathbf{p}_0$  to  $\Gamma_0$  (15), we obtain the quantity of interest to us:

$$\Gamma(\mathbf{p}_0) = \lambda/2 = vI/(vI\tau-1) \quad (19)$$

(a special symbol was introduced for it). The constant  $\tau$  is expressed in terms of a Watson integral<sup>5</sup>; for a SC lattice we shall use hereafter in the estimates the approximate value

$$\tau \approx 1/2. \quad (20)$$

We can now use the known results.<sup>3-4</sup> First the energy. We express the interaction energy  $\mathcal{E}_i$  for a given number of particles as follows:

$$\frac{\mathcal{E}_i}{N} = \frac{1}{2} \lambda \rho^2 \left[ 1 + \frac{16}{15\pi^2} (m\lambda)^{1/2} \rho^{1/2} \right], \quad (21)$$

where  $\rho \ll 1$  is the number of particles per site (the small parameter of the problem); we disregard henceforth the correction term in (21). We obtain the number of particles together with the energy from the condition for the minimum of expression for the total energy

$$\mathcal{E}/N = 1/2 \lambda \rho^2 - \mu \rho, \quad \mu = H_c - H, \quad (22)$$

where  $\mu$  is the energy of a single particle at the minimum of the band [see (10)]. The condition for the minimum of (22) yields

$$\rho = \frac{\mu}{\lambda}, \quad \frac{\mathcal{E}}{N} = \frac{-\mu^2}{2\lambda}. \quad (23)$$

The excitation spectrum is determined in the usual manner. We present the result for an excitation energy  $E(k)$ ; the spectrum takes near the minimum the form

$$E(k) = \left\{ \left( \frac{k^2}{2m} + \mu \right)^2 - \mu^2 \right\}^{1/2}, \quad (24)$$

and coincides with  $(\varepsilon - \varepsilon_0)$  far from the minimum. The quantity  $\mathbf{k}$  is the quasimomentum reckoned from the value  $\mathbf{p}_0$  at the minimum; it has the meaning of the excitation quasimomentum. The spectrum is linear at small  $k$ , as is usual in an antiferromagnet. In the present case the physical meaning of such a dependence is understandable: long-wave excitations correspond to acoustic oscillations of the considered magnon gas (with the "bare" spectrum (10)). We note that owing to the condition (23) on the density the interaction  $\lambda$  is not contained at all in the result (24).

We now consider a state with a particle flux, i.e., a moving condensate, wherein the particles are accumulated not at the band minimum  $\mathbf{p}_0$ , but at another point  $\mathbf{q} + \mathbf{p}_0$ . In this case the expression (22) for the energy is changed because the energy of a single particle is not  $-\mu$  but  $-\mu + q/2m$ ; we must accordingly put in (23)  $\mu \rightarrow \mu - q^2/2m$ . The excitation spectrum  $E$  near the minimum is given by

$$E(\mathbf{k}) = \frac{\mathbf{k}\mathbf{q}}{m} + \left\{ \left[ \frac{k^2}{2m} + \left( \mu - \frac{q^2}{2m} \right) \right]^2 - \left( \mu - \frac{q^2}{2m} \right)^2 \right\}^{1/2}, \quad (25)$$

and far from the minimum it coincides as before with  $(\varepsilon - \varepsilon_0)$ . Naturally, (25) is reminiscent of the spectrum of an ordinary Bose gas with a flux, the only difference is the appearance of a dependence on  $q$  under the square root in (25). The reason is that the quantity specified in our problem is not the number of particles but the quantity  $\mu$ , which assumes the role of the chemical potential.

The excitation spectrum remains thus stable ( $\tilde{E} > 0$ ) at sufficiently low velocities. If furthermore the system energy is independent of the phase of the condensate wave function, as in (22), we can speak of superfluidity. We shall return to this question in Sec. 4.

Now concerning the spin structure. One might seemingly be able to conclude that the system is not divided into sublattices, since the mean values of the operators  $S_{nx}$  and  $S_{ny}$  over a state with a fixed number of particles are zero. This is actually not so. A perturbation linear in  $\beta$  and  $\beta^+$  alters this conclusion<sup>6</sup> (such a perturbation is apparently always present because of crystal-lattice imperfections). As a result, the mean values of  $S_{nx}$  and  $S_{ny}$  differ from zero. They are expressed in terms of the mean values of the operators  $\beta_n$  and  $\beta_n^+$  [Eq. (2)], which are determined in the principal approximation, just as in an ideal Bose gase, by the operators  $\beta_{p_0}$  and  $\beta_{p_0}^+$  replaced by the numbers

$$\beta_{p_0} \rightarrow (N\rho)^{1/2} e^{i\varphi}$$

( $\varphi$  is an arbitrary phase). Thus, in the considered case of one minimum of  $\varepsilon(\mathbf{p})$  in the band we obtain a state with two sublattices. It might seem that we have returned to the classical picture. The angle between the spin and the magnetic field, however, is given by the value (23) of  $\rho$  as specified by us and differs greatly from the classical result (see the next section).

We note that the spin structure is actually included in the condensate wave functions (details in Sec. 4).

### 3. COMPARISON WITH THE QUASICLASSICAL APPROACH

We compare here our results with those obtained by the traditional approach.<sup>1</sup> We recall briefly the procedure and the results of each stage (classical approach, quadratic Hamiltonian) and take also the interaction into account.

We consider an antiferromagnet with two sublattices, and perform the calculations for SC and *bcc* lattices with nearest-neighbor interaction.

We begin, as usual by rewriting the Hamiltonian (1), introducing explicitly for each sublattice its own quantization axis. We transform to a new coordinate frame 1, 2, 3 by rotating the  $x, y, z$  frame about the axis through an angle  $\pm\theta$ , depending on the sublattice (the 2 axis coincides with  $y$ ). In the new coordinates, the Hamiltonian (1) takes the form

$$\begin{aligned} \mathcal{H} = & \frac{1}{2} \sum_{n \neq n'} I_{nn'} \{ (S_{n3}S_{n'3} + S_{n1}S_{n'1}) \cos 2\theta + S_{n2}S_{n'2} \\ & + (\sin 2\theta_n - \sin 2\theta_{n'}) S_{n1}S_{n'3} \} + H \sum_n (S_{n3} \cos \theta - S_{n1} \sin \theta_n), \end{aligned} \quad (26)$$

where  $\theta_n = \pm \theta$ , depending on the sublattice, and the operators  $S_{n1}$ ,  $S_{n2}$ , and  $S_{ns}$  are, as before, Pauli matrices multiplied by 1/2.

The first stage is the classical approximation: we replace in (26) the operators by numbers,  $S_{n3} \rightarrow -1/2$ ,  $S_{n1} = S_{n2} \rightarrow 0$  (independently of the number of the site), and find the minimum with respect to  $\theta$ . This yields

$$\cos \theta = H/H_c. \quad (27)$$

We express the energy in a form that can be compared with (23), i.e., subtracting  $\varepsilon_0(\mathbf{H})$ , see (4), we obtain

$$\mathcal{E}'/N = -\mu^2/2\lambda', \quad \lambda' = 2\sqrt{I}. \quad (28)$$

It is easy to verify that  $\lambda' > \lambda$ ; thus, for an SC lattice, taking (20) into account, we have  $\lambda' \approx 2\lambda$ .

The energy of the gas phase with the Bose condensate is thus substantially lower, and the magnetic susceptibility is higher (double for the SC lattice). This means that the classical picture cannot reveal the main contribution to the energy near  $H_c$ .

One might object that the principal quantity  $\mathcal{E}_0(H)$  is given by the classical approach with only a small error. The representation of the energy in the form (22), however, is in fact a Landau expansion in the small parameter  $\rho$  near a second-order phase transition (the transition point is  $H = H_c$ ); a quantitative theory must of course, yield the coefficients of this expansion. It should be noted that the classical approach the usual calculation method in similar situations. One example—displacive transitions in crystals when the phonon spectrum contains the so-called “soft mode.” The role of the soft mode in an antiferromagnet is laid by the magnon spectrum (10) in the vicinity of the minimum. In the above-mentioned crystals the order parameter is chosen to be the classical sublattice displacement; the analog in an antiferromagnet is the deflection of the spins from the z axis. Nonetheless, the classical theory is found to be insufficient. The reason is clear: the classical approach is equivalent here to the self-consistent field approximation, which does not take the correlation effects into account (in our approach, see Sec. 2, the pair correlations are taken into account by a transition to the total scattering amplitude). There is hope therefore that allowance for the quantum fluctuations will improve matters, and so it does.

The next stage is allowance for the quantum fluctuations within the framework of a quadratic Hamiltonian. The particle operators can be introduced by changing over in (25) to the Pauli operators (2) (where  $x, y, z$  must be taken to mean 1, 2, 3). As usual, the terms linear in  $\beta$  and  $\beta^+$  vanish because of condition (27). That part of the Hamiltonian (25) which is quadratic in these operators is of the form

$$\begin{aligned} \mathcal{H}_2 = & \frac{\nu I}{2} \sum_n \beta_n^+ \beta_n + \left( \frac{H}{H_c} \right)^2 \cdot \frac{1}{2} \sum_{n \neq n'} I_{nn'} \beta_n^+ \beta_{n'} \\ & - \frac{1}{2} \left[ 1 - \left( \frac{H}{H_c} \right)^2 \right] \cdot \frac{1}{2} \sum_{n \neq n'} I_{nn'} (\beta_n \beta_{n'} + \text{H.a.}). \end{aligned} \quad (29)$$

Near  $H_c$ , the last term of (29) is small, so that conditions (3) can be disregarded and  $\beta$  and  $\beta^+$  can be regarded as Bose operators. We transform in (29) to quasimomenta and dia-

gonalize this operator. The contribution to the energy is

$$\frac{\langle \mathcal{H}_2 \rangle}{N} = -\frac{\mu^2}{2\nu I} \left( \frac{\nu I \tau}{2} - 1 \right) \quad (30)$$

(the angle brackets in this section denote averaging over the ground state of the Hamiltonian (29), i.e., over the quasiparticle vacuum). The sum of (28) and (30) is exactly (23).

The quasiparticle spectrum obtained by diagonalizing (29) agrees near  $H_c$  with the spectrum obtained in Sec. 2.

The following must be noted here. The magnetic susceptibility can be calculated using expression (23) for the energy. On the other hand, we can calculate first the mean value  $\langle S_{nz} \rangle$  and from it the susceptibility; this turns out to be equivalent to calculating with the aid of expression (28) for the energy. The results are substantially different: this means that the state obtained in the traditional approach (classical treatment plus a quadratic Hamiltonian) is not an eigenstate and differs from it greatly (for an eigenstate we would have an equality, see Eqs. (11) and (16) of Ref. 7). This is not surprising, for an interaction that cannot be neglected in this case was not taken into account.

To verify this, consider the unaccounted-for part (of third and fourth order in  $\beta$  and  $\beta^+$ ) of the Hamiltonian (26):

$$\begin{aligned} \mathcal{H}_3 = & \frac{1}{4} \sum_{n \neq n'} I_{nn'} (\beta_n + \beta_{n'}) \beta_{n'}^+ \beta_n^+ (\sin 2\theta_{n'} - \sin 2\theta_n) \\ & + \left[ 2 \left( \frac{H}{H_c} \right)^2 - 1 \right] \cdot \frac{1}{2} \sum_{n \neq n'} I_{nn'} \beta_n^+ \beta_{n'}^+ \beta_{n'} \beta_n. \end{aligned} \quad (31)$$

For a rough estimate of the contribution of this operator we can simply average it over the vacuum of the quasiparticles. In this case only the second term of (31) operates, while the principal contribution near  $H_c$ , i.e., the one proportional to  $\mu^2$ , is made by the anomalous mean values:

$$\langle \mathcal{H}_3 \rangle \approx \frac{1}{2} \sum_{n \neq n'} I_{nn'} \langle \beta_n^+ \beta_{n'}^+ \rangle \langle \beta_{n'} \beta_n \rangle.$$

We present the final result:

$$\frac{\langle \mathcal{H}_3 \rangle}{N} = \frac{\mu^2}{2\nu I} \left( 1 - \frac{\nu I \tau}{2} \right)^2. \quad (32)$$

As for the contribution of the first term in (31), its estimated value in second-order perturbation theory yields the small value  $\sim \mu^{5/2}$  (in analogy with the correction term in (21)).

The resultant energy, i.e., the sum of (28), (30), and (32), turns out thus to be higher than (23) for the gas phase with a Bose condensate (by approximately 25% for an SC lattice, see (20)). This to be expected, for there can be nothing but a gas in this situation.

It appears that if it were possible to solve rigorously the problem with the Hamiltonian  $\mathcal{H}_2 + \mathcal{H}_3$ , as well as with condition (3), the state obtained would coincide with that considered in Sec. 2. It goes without saying that this approach is not simple, whereas the analogy with the gas leads directly to the goal.

## 6. DISCUSSION

Let us summarize. The analogy with the gas permits a correct account to be taken of the correlation effects, or more

accurately, of pair correlations. The problem is reduced to calculation of the interaction constant  $\lambda$  that determined the energy and the magnetic susceptibility. The exchange interaction enters also via the effective mass  $m$  on which the excitation spectrum depends; in the general case  $m$  is a tensor.

Knowing  $\lambda$  we can find also other characteristics, e.g., the transition temperature  $T_c$ . Let us consider a state above the transition point (without a condensate). The particle interaction energy  $\mathcal{E}'_i$  in this phase is given by the expression

$$\mathcal{E}'_i/N = \lambda \rho^2.$$

This means that the particle energy shift due to the interaction is  $2\lambda\rho$ ; this value (with opposite sign) can be regarded as an increment to the quantity  $\mu$  that plays the role of the chemical potential; the considered state is stable when the effective chemical potential ( $\mu - 2\lambda\rho$ ) is negative:

$$\mu - 2\lambda\rho \leq 0. \quad (33)$$

Its vanishing gives the Bose-condensation point. For the isotropic minimum we obtain hence

$$T_c \approx 2,087 m^{-1} (\mu/\lambda)^{2/3}.$$

This is the sought transition curve in the  $(T, H)$  plane in the case of a second-order transition.

At the transition point  $\rho = \mu/2\lambda$ , see (33). It is interesting to note that the number of particles from the transition point increases (the magnetization decreases) both with rising and with dropping temperature [ $\rho = \mu/\lambda$ ] at absolute zero, see (23)].

The analogy with the gas yields one other important characteristic—the periods of the spin structure. It is easily seen that these periods are determined by the coordinates of the minima of the function  $\varepsilon(\mathbf{p})$  (6). Without touching on the case, trivial in this sense, of a single minimum (Fig. 2), let us explain this using another, likewise simple, example, the more so since it is of interest on its own. Namely, we consider the case of two minima of  $\varepsilon(\mathbf{p})$  in the band; we denote the coordinates of the minima by  $\pm \mathbf{p}_0$  (now  $\mathbf{p}_0$  is not on the boundary of the band). This situation is possible in a uniaxial crystal. The system energy is written in the form

$$\mathcal{E}/N = \frac{1}{2}\lambda_1(\rho_1^2 + \rho_2^2) + \lambda_2\rho_1\rho_2 - \mu(\rho_1 + \rho_2), \quad (34)$$

where  $\rho_1$  and  $\rho_2$  are the particle numbers per site in valleys 1 and 2. In this case there are two types of interaction: between particles of the same valley, and between particles from different valleys; accordingly, two interaction constants appear,  $\lambda_1$  and  $\lambda_2$ . Equation (34) is a direct generalization of (22) to this case.

Minimization of (34) is meaningful only under the condition

$$\lambda_1 > 0, \quad \lambda_1 + \lambda_2 > 0.$$

States of two types are possible:

$$1) \lambda_1 < \lambda_2; \rho_1 = \rho = \mu/\lambda_1, \rho_2 = 0 \text{ (or vice versa)},$$

$$\mathcal{E}_1/N = -\mu^2/2\lambda_1.$$

$$2) \lambda_1 > \lambda_2; \rho_1 = \rho_2 = \rho' = \mu/(\lambda_1 + \lambda_2).$$

$$\mathcal{E}_2/N = -\mu^2/(\lambda_1 + \lambda_2).$$

We have here, as it were, a mixture of two gases, and the first case corresponds to stratification of the phases. Within the confines of one phase (domain) we obtain in the principal approximation

$$\begin{aligned} \langle \beta_n \rangle &= \sqrt{\rho} \exp \{ \pm i(\mathbf{p}_0 \mathbf{R}_n + \varphi) \}, \quad \langle S_{nz} \rangle \\ &= -\frac{1}{2} + \rho, \quad \langle S_{nx} \rangle = \sqrt{\rho} \cos(\mathbf{p}_0 \mathbf{R}_n + \varphi), \\ \langle S_{ny} \rangle &= \mp \sqrt{\rho} \sin(\mathbf{p}_0 \mathbf{R}_n + \varphi), \end{aligned}$$

where  $\varphi$  is an arbitrary phase. The spin structure in this case is a right- or left-hand helix, depending on the type of domain (the different signs in the expressions).

In the second (one-domain) case we obtain a spin structure of the fan type

$$\begin{aligned} \langle \beta_n \rangle &= \sqrt{\rho'} \{ \exp [i(\mathbf{p}_0 \mathbf{R}_n + \varphi_1)] + \exp [i(-\mathbf{p}_0 \mathbf{R}_n + \varphi_2)] \}, \\ \langle S_{nz} \rangle &= -\frac{1}{2} + 4\rho' \cos^2 \left[ \mathbf{p}_0 \mathbf{R}_n + \frac{\varphi_1 - \varphi_2}{2} \right], \\ \langle S_{nx} \rangle &= 2\sqrt{\rho'} \cos \left[ \mathbf{p}_0 \mathbf{R}_n + \frac{\varphi_1 - \varphi_2}{2} \right] \cos \frac{\varphi_1 + \varphi_2}{2}, \\ \langle S_{ny} \rangle &= -2\sqrt{\rho'} \cos \left[ \mathbf{p}_0 \mathbf{R}_n + \frac{\varphi_1 - \varphi_2}{2} \right] \sin \frac{\varphi_1 + \varphi_2}{2}. \end{aligned}$$

In this case the solution contains two arbitrary phases corresponding to two non-phased condensates. We note that the spin-structure periods are generally speaking incommensurate with the initial-lattice periods.

It can be seen from the foregoing expression that both the periods and the type of the spin structure are determined. Something similar occurs also in the arbitrary case. This example is of interest also because it reveals a rare case of condensates that are independent in phase. In the general case the phase differences are fixed by the minimum-energy conditions.

So far we have considered an isotropic case. Uniaxial magnetic anisotropy does not change anything significantly if the magnetic field is parallel to the axis. Actually, in this case there exists as before a good quantum number—the projection of the total spin on the magnetic-field direction; the total number of particles is correspondingly preserved. The analogy with the Bose gas remains therefore in force.

As for arbitrary directions of the magnetic field and of the anisotropy axis, we note only one thing: even at arbitrarily small anisotropy transverse to the field, the leeway in the condensate wave-function phase is lost (the so-called fixing of the phase takes place), and with it also the superfluidity property.

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