

# Phase transition describable by self-consistent-field theory in an exactly solvable model

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The mechanism of indirect interaction of the order parameter via acoustic oscillations is considered. The special character of the contribution of the static deformation is taken into account. The spectrum of the acoustic oscillations that interact with the order parameter is assumed to be linear. The microscopic description of the thermodynamics with the aid point transformations is reduced to the self-consistent field theory. The principal results of the theory are applied to the model in question. The low-temperature phase transition in  $\text{KMnF}_3$  is discussed on the basis of these results.

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## INTRODUCTION

In the theory of phase transitions, the interaction of the order parameter with the mean field is usually considered only as an approximate description of the initial localized microscopic interaction.<sup>1</sup> At the same time, the interaction with the mean field is actually the result of the special character of the contribution of the homogeneous mode to the indirect exchange.<sup>1)</sup> In the present paper we investigate the case when the total interaction reduces entirely to the interaction of the order parameter with the mean field.

The simplest physical system that has such a behavior is a system of two-level states placed in an elastically isotropic medium and interacting only with the deformation. The effective interaction is made up of the contribution of the static deformation and of the exchange via acoustic oscillations. The linearity of the spectrum of the acoustic oscillations, which is typical of the model, leads to the absence of a short-range dynamic effective interaction. The model can be solved exactly and represents the case when the self-consistent field theory yields a rigorous description of the thermodynamics in the microscopic approach. The model includes a first-order phase transition. In the temperature-pressure plane, the transition line terminates at the critical point. Two possible critical behaviors appear in the model. If the degree of degeneracy of the levels of the two-level system are different van der Waals behavior takes place near the critical point. If the degrees of degeneracy of the levels coincide, the results correspond to the Weiss theory.<sup>5</sup> The low-temperature phase transition recently observed in

$\text{KMnF}_3$  (Ref. 6) is interpreted as a direct realization of the model.

## DESCRIPTION OF MODEL

Assume that a lattice with two-level systems at its site is immersed in a homogeneous elastically isotropic medium. The Hamiltonian of such a composite system can be written in the form

$$H = \int \left( \frac{\lambda}{2} U_{\alpha\alpha}^2(r) + \mu U_{\alpha\beta}^2(r) \right) dV + \sum_j (J_0 + gU_{\alpha\alpha}(r_j)) \eta_j, \quad (1)$$

where  $\lambda$  and  $\mu$  are the elastic moduli,  $U_{\alpha\beta}(r)$  is the strain tensor at the point  $r$ , summation over repeated indices is implied,  $\eta_j = \pm 1$  is a parameter that specifies the occupation of the states of the two-level system with coordinate  $r_j$ , and  $J_0 + gU_{\alpha\alpha}(r_j)$  is the difference between the level energies of the two-level system and depends on the strain. The summation in (1) is over the lattice sites, and the integration is over the corresponding volume.

Allowance of the deformation contribution to the thermodynamics will be carried out in analogy with Ref. 7. We determine the expansions of the strain tensor and of the parameter  $\eta_j$  in Fourier harmonics by the formulas

$$U_{\alpha\beta}(r) = \bar{U}_{\alpha\beta} + \frac{i}{2V^{1/2}} \sum_{\mathbf{k}} (k_\alpha U_\beta^k + k_\beta U_\alpha^k) e^{i\mathbf{k}r}, \quad (2)$$

$$\eta_j = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} \eta_{\mathbf{k}} \exp(i\mathbf{k}r_j). \quad (3)$$

Here  $\bar{U}_{\alpha\beta}$  is the uniform deformation,  $U_\beta^k$  is the Fourier component of the displacement vector,  $V$  is the volume

of the system, and  $N$  is the total number of lattice sites. In expression (2), the summation is over a denumerable set of values of  $\mathbf{k}$ , and the prime of the summation sign means omission of the term with  $\mathbf{k}=0$ . The number of terms in the sum (3) is finite (equal to  $N$ ), and the sum runs over the same values of  $\mathbf{k}$  as in the long-wave part of the denumerable set of values in (2) (this is accomplished by a suitable choice of the boundary condition).

We consider the thermodynamic potential

$$\Phi = -T \ln \sum_{\dots} \{ \exp(-\beta H + \beta V \sigma_{\alpha\beta} \bar{U}_{\alpha\beta}) \}, \quad (4)$$

where  $\sigma_{\alpha\beta}$  is the stress tensor,  $T=1/\beta$  is the temperature, and the sum is taken over the configurations.

We substitute in (4) expression (1) and take (2) and (3) into account. Next, following Ref. 8, we separate formally the contributions of the "bare" acoustic oscillations, a procedure which is statistically accurate. Expression (4) then takes the form

$$\Phi = V \left( \frac{\lambda}{2} \bar{U}_{aa}^2 + \mu \bar{U}_{\alpha\beta}^2 - \sigma_{\alpha\beta} \bar{U}_{\alpha\beta} \right) + \Phi_{ac} - T \ln \sum_{\dots} \left\{ \left\langle \exp \left[ -\beta (J_0 + g \bar{U}_{aa}) \sum_j \eta_j - \frac{i\beta g}{v^{1/2}} \sum_{\mathbf{k}} (kU^{\mathbf{k}}) \eta_{-\mathbf{k}} \right] \right\rangle_{ac} \right\}. \quad (5)$$

Here  $v=V/N$  is the volume of the lattice cell,

$$\Phi_{ac} = -T \ln \sum_{\dots} \{ \exp(-\beta H_{ac}) \}, \quad (6)$$

$$H_{ac} = \frac{\lambda+2\mu}{2} \sum_{\mathbf{k}} |(kU^{\mathbf{k}})|^2 + \frac{\mu}{2} \sum_{\mathbf{k}} (k^2 |U^{\mathbf{k}}|^2 - |(kU^{\mathbf{k}})|^2) \quad (7)$$

are respectively the thermodynamic potential and the Hamiltonian of the acoustic oscillations. The angle brackets in (5) denote averaging over the acoustic oscillations.

After averaging the exponential in (5), the first term in the exponent remains unchanged, and the second, by virtue of the Gaussian character of the distribution of the acoustic oscillations, can be reduced to the form<sup>2)</sup>

$$\frac{\beta g^2}{2v(\lambda+2\mu)} \sum_{\mathbf{k}} |\eta_{\mathbf{k}}|^2. \quad (8)$$

Adding to (8) the corresponding term with  $\mathbf{k}=0$ , we transform the sum over  $\mathbf{k}$  into a sum over the sites of  $\eta_j^2$ . Since, by definition,  $\eta_j^2=1$ , this sum leads to a constant increment to the thermodynamic potential.

To transform the square of the zeroth harmonic, which compensates the increment to the sum (8), we use the statistical identity<sup>8)</sup>

$$\sum_{\dots} \left\{ \exp \left[ L \left( \frac{1}{N} \sum_j \xi_j \right) \right] \right\} = \exp \left[ L(\langle \xi \rangle) - \frac{dL(\langle \xi \rangle)}{d\langle \xi \rangle} \langle \xi \rangle \right] \times \sum_{\dots} \left\{ \exp \left[ \frac{dL(\langle \xi \rangle)}{d\langle \xi \rangle} \frac{1}{N} \sum_j \xi_j \right] \right\}, \quad (9)$$

where  $L(Z)$  is an arbitrary differentiable function,  $\xi_j$  is an arbitrary local function of the configuration, and the partition function, which determines the mean values, is specified by the last factor in the right-hand side of (9).

The homogeneous deformation  $\bar{U}_{\alpha\beta}$  is determined from the condition of the minimum of the potential  $\Phi$ . Assuming for simplicity that an isotropic pressure has been applied to the system ( $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta}$ ), we obtain for the homogeneous-deformation tensor the expression

$$\bar{U}_{\alpha\beta} = -\frac{1}{3} \left( \frac{p}{K} + \frac{A}{v} \langle \eta \rangle \right) \delta_{\alpha\beta}, \quad (10)$$

where  $K = \lambda + 2\mu/3$  is the modulus of the hydrostatic compression and  $A = g/K$ .

Using the transformations listed above and the results of (8)–(10), we obtain for the thermodynamic potential

$$\Phi = \Phi_0 + \frac{N}{2} G \langle \eta \rangle^2 - T \ln \sum_{\dots} \left\{ \exp \left( \beta J \sum_j \eta_j \right) \right\}, \quad (11)$$

where

$$\Phi_0 = \Phi_{ac} - \frac{p^2 V}{2K} - \frac{g^2 N}{2v(\lambda+2\mu)}, \quad (12)$$

$$G = \frac{g^2}{v} \left( \frac{1}{K} - \frac{1}{\lambda+2\mu} \right) = \frac{2g^2(1-2\sigma)^2}{vE(1-\sigma)}, \quad (13)$$

$$J = Ap - J_0 + G \langle \eta \rangle. \quad (14)$$

For convenience we present here also the expression of  $G$  in terms of Young's modulus  $E$  and the Poisson coefficient  $\sigma$ .<sup>9)</sup>

Thus, the initial interaction has been reduced to an interaction of the parameter  $\eta_j$  with effective field  $J$ . The sum over the configurations can now be easily calculated. The expressions for the thermodynamic potential and for the average value of the order parameter take a final form

$$\Phi = \Phi_0 + \frac{1}{2} NG \langle \eta \rangle^2 - TN \ln [2(q_+ q_-)^{1/2} \text{ch } x], \quad (15)$$

$$\langle \eta \rangle = \text{th } x. \quad (16)$$

Here  $q_+$  and  $q_-$  are the degrees of degeneracy of the states of the two-level system with  $\eta=1$  and  $\eta=-1$ , respectively, and  $a = q_+/q_-$ . We have also introduced the notation  $x_0 = -(\frac{1}{2}) \ln a$  and  $\beta J = x_0 + x$ .

## SOLUTION IN THE CASE OF ARBITRARY $a \neq 1$

From (14) and (16) we obtain an equation for the self-consistent value

$$T(x_0 + x) - A(p - p_0) = G \text{th } x, \quad (17)$$

where  $p_0 = J_0/A$ . The ambiguity of the stable solution of Eq. (17) leads to a first-order phase transition in the system. Taking into account the symmetry of (15) with respect to the change of the sign of  $x$ , we obtain from (17) an equation for the equilibrium phase transition line

$$p_{tr} = p_0 + \frac{T}{A} x_0. \quad (18)$$

The phase-transition line terminates at a critical point with parameters

$$T_c = G, \quad p_c = p_0 + \frac{G}{A} x_0. \quad (19)$$

Finally, the limits of the regions of stability of the metastable states are determined in accordance with

(17) by the equation

$$A(p-p_0) = \pm \left( GR + \frac{T}{2} \ln \frac{1-R}{1+R} \right), \quad (20)$$

where the pressure  $p_0$  is given by the condition (18),  $R = (1 - T/G)^{1/2}$ , and the choice of the sign (upper or lower) determines one of two branches of the boundary curve. The corresponding phase diagram in the  $(p, T)$  plane is shown in Fig. 1a.

The discontinuities of the entropy and of the volume in an equilibrium phase transition are determined by the modulus of the order parameter:

$$\left| \left[ \frac{\Delta V}{N} \right] \right| = 2|A\langle \eta \rangle|, \quad \left| \left[ \frac{\Delta S}{N} \right] \right| = 2|x_0\langle \eta \rangle|. \quad (21)$$

For the isothermal compressibility and the specific heat we obtain from (14)–(16) the expressions

$$-\frac{1}{V} \frac{\partial^2 \Phi}{\partial p^2} = \frac{1}{K} + \frac{\beta A^2}{v} \chi, \quad (22)$$

$$c_p = c_{p0} + (\beta J)^2 \chi, \quad (23)$$

where

$$\chi = \frac{1 - \langle \eta \rangle^2}{1 - \beta G(1 - \langle \eta \rangle^2)}, \quad (24)$$

$c_{p0}$  is the regular part of the specific heat and is obtained by differentiating  $\Phi_0$ .

At the boundary of the stability region, the denominator  $\chi$  in (24) vanishes, and this leads to a divergence of the thermodynamic derivatives, as should be the case. Special properties are possessed by the extremum point of the stability limit (the point  $M$  in Fig. 1a), whose coordinates are

$$T_M = \frac{4aG}{(a+1)^2}, \quad p_M = p_0 - \frac{G}{A} \frac{a-1}{a+1}. \quad (25)$$

At this point we have  $J=0$ . Therefore, in contrast to the other points of the stability-region boundary, the specific heat  $c_p$  remains finite on moving to this point from the metastability region, and tends to the value  $c_{p0}$ .

The phase-transition line is a cut through the  $(p, T)$

plane of the stable states. The critical point is in this case a branch point, so that the behavior of the thermodynamic quantities as they approach this point does not depend on the character of the approach. Introducing the distance to the critical point  $\varepsilon$  and the approach angle  $\varphi$  by the relations

$$\frac{T-T_c}{G} = \varepsilon \cos \varphi, \quad \frac{A(p-p_0)}{G} = \varepsilon \sin \varphi, \quad (26)$$

we obtain, for example for  $\chi$  in the vicinity of the critical point the expression

$$\chi^{-1} = \Xi \varepsilon \cos \varphi. \quad (27)$$

The function  $\Xi$  is defined by the formulas

$$\Xi = [2\Lambda + 1 + 2(\Lambda^2 + \Lambda)^{1/2}]^{1/2} + [2\Lambda + 1 - 2(\Lambda^2 + \Lambda)^{1/2}]^{1/2} - 1 \quad (28a)$$

at  $\Lambda < -1$  or  $\Lambda > 0$

$$\Xi = 1 - 4 \cos^2 \left[ \frac{1}{3} \arctg \left( \frac{\Lambda+1}{-\Lambda} \right)^{1/2} \right] \quad (28b)$$

at  $-1 < \Lambda < 0$ , where

$$\Lambda = \frac{9(\operatorname{tg} \varphi - x_0)^2}{4\varepsilon \cos \varphi}. \quad (29)$$

When the critical point is approached, the singularity has a power-law character, but the exponent in the dependence on the trajectory of the motion can vary in the range from  $\frac{2}{3}$  to 1.

On the family of trajectories corresponding to a definite value of the exponent, we have  $\chi = b\varepsilon^{-\alpha}$ , where  $b$  is a parameter of the family. The family itself is given at  $\varepsilon \ll 1$  and  $\frac{2}{3} < \alpha < 1$  by the equation

$$\varepsilon^{(3\alpha-2)/2} = \pm 3b^{2/3} (1+x_0^2)^{1/2} (\varphi - \varphi_0). \quad (30)$$

Here and below, at  $T > T_c$ , we choose  $\varphi_0$  to be the angle of inclination of the phase-transition line to the temperature axis, and at  $T < T_c$  the angle  $\varphi_0$  differs from the transition-line inclination angle by  $\pi$ .

The case  $\alpha=1$  in the limit  $\varepsilon \ll 1$  corresponds to trajectories along which  $\Lambda$  is constant. The expression for  $b$  in the trajectory equation takes the form

$$b = (1+x_0^2)^{1/2} |\Xi|^{-1}, \quad (31)$$

$$\varepsilon^{1/2} = \pm \frac{3(1+x_0^2)^{1/2}}{2|\Lambda|^{1/2}} (\varphi - \varphi_0). \quad (32)$$

This case covers also the motion along the phase-transition line ( $\varphi = \varphi_0$ ), in accord with the van der Waals theory.<sup>1</sup>

Motion along trajectories with constant angles  $\varphi \neq \varphi_0$  corresponds to the other limiting value of the exponent:  $\alpha = \frac{2}{3}$ . In this case

$$b = |3 \sin \varphi - 3x_0 \cos \varphi|^{-1/2}. \quad (33)$$

#### THE SYMMETRIC CASE $a=1$

If  $a=1$ , then  $x_0=0$ , so that the phase-transition line is determined by the condition  $p=p_0$ . The corresponding phase diagram is shown in Fig. 1b. The entropy jump

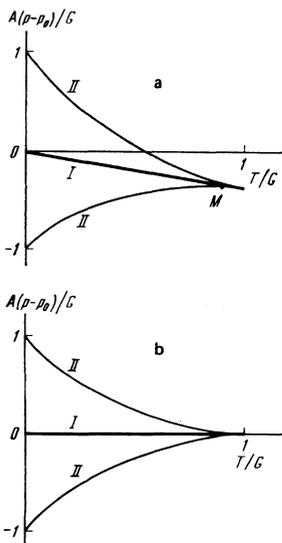


FIG. 1. Phase diagrams: a—case  $a=2$ , b—symmetric case  $a=1$ ; I—phase-transition line, II—limits of stability of metastable regions.

in the equilibrium phase transition is equal to zero in accord with (21).

Let us examine the behavior of the specific heat  $c_p$  in the vicinity of the critical point when  $a=1$ . Figure 2 shows the behavior of the irregular part of the specific heat in the metastable region at fixed pressures, as a function of the parameter  $\tau = T/T_p - 1$ , where  $T_p$  is the temperature instability at the considered pressure  $p$ . In the case  $p = p_0$  (line 1 of Fig. 2) the specific heat has a finite limit as  $\tau \rightarrow 0$ . If  $|p - p_0| \neq 0$  (curves 2 and 3), the heat capacity diverges like  $|\tau|^{-1}$ . In this case the region of considerable deviation of the specific heat from the case  $p = p_0$  is determined by the condition  $|\tau| \ll |A(p - p_0)/G|^{2/3}$ .

In the case of motion in the stable region, the value of the heat capacity at the critical point, remaining finite, depends on the character of the approach, as determined by the expression

$$c_p = c_{p_0} + 1 - \Xi^{-1}, \quad (34)$$

where  $\Xi$  is given by formulas (28), and the corresponding expression for  $\Lambda$  takes in accord with (29) the form

$$\Lambda = \frac{9 \sin^2 \varphi}{4e \cos^3 \varphi}. \quad (35)$$

It follows from (34) that the most interesting are the trajectories along which  $\Lambda$  is constant. In this case the specific heat has at the critical point a definite value that depends on  $\Lambda$ . The difference  $c_p - c_0$  as a function of  $\Lambda^{-1}$  is shown in Fig. 3. In particular, for motion along the trajectory  $p = p_0$  we obtain the usual specific-heat discontinuity of the self-consistent-field theory.<sup>1</sup>

We note finally that in the case of motion along isobars that far from the phase-transition line, the thermodynamic quantities have in accordance with (12)–(16) the singularities usually obtained for an ensemble of two-level systems (the Schottky anomalies) at all values of  $a$ .

## CONCLUSION

The considered model is an ordered system whose thermodynamics is described exactly by the theory of the self-consistent field. In real systems there exist also interaction that depend on the distance.<sup>3)</sup> To the

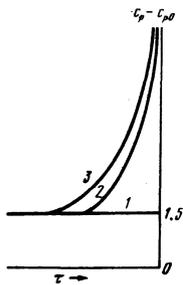


FIG. 2. Behavior of the irregular part of the specific heat  $c_p - c_{p_0}$  in the metastability region, near the critical point, in the case  $a=1$ . Line 1 corresponds to the pressure  $p_1 = p_0$ . Curves 2 and 3 correspond to  $|p_3 - p_0| > |p_2 - p_0| \neq 0$ .

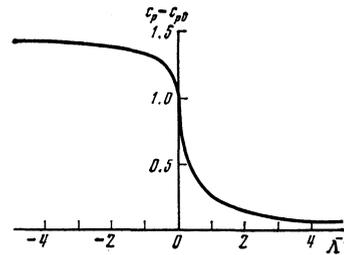


FIG. 3. Dependence of the irregular part of the specific heat  $c_p - c_{p_0}$  at the critical point on the trajectory parameter  $\Lambda^{-1}$ .

extent that these interactions are small, the mechanism investigated in the present paper can be the reason why the experimentally observed behavior was close to the self-consistent behavior (for other possible causes see footnote 1).

The described simplest model can be directly applied, for example, to the case of an isomorphic transition, when the pressure-induced growth of the crystal field causes the molecular levels to cross, so that the ground state is altered thereby. To be able to regard such a system as a two-level system, the corresponding temperature must be low enough.

A characteristic feature of the self-consistent behavior is the suppression of the fluctuations by the mean field, so that it becomes possible to approach the boundary of the stability region in experiment. In this connection, we point out the phase transition recently observed by Strauss and Riederer<sup>6</sup> in  $\text{KMnF}_3$  at 1.7 K at a uniaxial pressure 197 kbar. According to their data, the low-pressure phase was preserved up to 2.35 kbar and was independent of the rate of change of pressure. They have also investigated the excitonic level possessed by  $\text{KMnF}_3$ . As a result of the phase transition, the position of the level changed jumpwise by  $51 \text{ cm}^{-1}$ . Finally, according to their conclusions, the phases of the high and low pressures are both tetragonal and all that differs in their structure is the tetragonality factor.

We present an estimate for this transition on the basis of the results of the present paper. We choose the elastic parameters to be  $K = 0.6 \text{ Mbar}$  and  $\lambda + 2\mu = 1 \text{ Mbar}$ .<sup>10</sup> Recognizing that the stress tensor is of the form  $\sigma_{\alpha\beta} = -p\delta_{\alpha\beta}$  (which leads to the substitution  $p \rightarrow p/3$  in the formulas of interest to us) and assuming the upper experimental value of the pressure to be located on the boundary of the stability region, we obtain from (20) the estimate  $g = 1.6 \times 10^{-13} \text{ erg}$ . Therefore the estimate for the change of the energy of the ground state in the phase transition is  $12 \text{ cm}^{-1}$ , which agrees in order of magnitude with the observed shift of the excitonic level. Assuming that the other conclusions of the present paper are qualitatively applicable for the description of the low-temperature transition to  $\text{KMnF}_3$ , we can, in particular, predict the existence of a critical point on the phase-transition line. An estimate of the position of the critical point yields a value  $T_c \approx 1.76 \text{ K}$ . An experimental check on this prediction, in our opinion, is of interest.

In conclusion, I am grateful to V. M. Nabutovskii for constant interest in the work. I am deeply grateful to V. L. Ginzburg for all the participants of the seminar

under his direction for a discussion. Finally, I take pleasure in thanking É. B. Amitin, A. I. Larkin, E. V. Matizen, and F. I. Khomskii for a discussion of the work.

- <sup>1</sup>This phenomenon is discussed in the Gehrings' review.<sup>2</sup> We emphasize that when the exchange is via acoustic phonons the total effect is due to the presence of a gap in the spectrum of the elastic fluctuations. We note also that the presence of the gap in the spectrum extends the region of validity of the Landau theory to cover the entire vicinity of the phase transitions.<sup>3,4</sup>
- <sup>2</sup>The separation of the contribution of the acoustic oscillations to the thermodynamic potential and the ensuing effective interaction in the form (8) correspond to diagonalization of the part of the Hamiltonian  $H$  with  $k \neq 0$ .
- <sup>3</sup>If the nonlinearity of the phonon spectrum is of importance to the short-wave part of the momenta corresponding to the considered lattice of two-level systems, then the effective interaction via the phonons also contains a contribution that depends on the distances between the lattice points.

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## Theory of dislocation retardation in antiferromagnets

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We investigate dislocation retardation in antiferromagnets as a result of "Cerenkov" generation of spin waves and their scattering by the moving dislocations, as a function of the ground state of the antiferromagnet. It is established that the retardation force has a velocity threshold in the magnon generation mechanism; the influence of the magnetic field on the threshold velocity is investigated. The dependence of the retardation force on the temperature, velocity, and orientation of the dislocation is studied. It is shown that in the presence of a non-activation branch in the spin-wave spectrum the retardation force is anomalously large. The general character of the temperature dependence of the retardation force of the dislocations in antiferromagnetic dielectrics and metals is investigated. It is shown that interaction with the spin waves can make a substantial contribution to the dislocation retardation force in antiferromagnets at low temperatures.

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### 1. INTRODUCTION

It is well known that many properties of solids (plasticity, brittle fracture, microhardness) and also some kinetic phenomena (sound absorption, internal friction, width of ferromagnetic resonance line, etc.) are determined by the dislocations in the crystal. At low temperatures, when the diffusion processes are suppressed, the principal role in the dislocation retardation is played by their interaction with the quasiparticles of the crystal. The interaction of dislocations with phonons and conduction electrons has been sufficiently well investigated (see, e.g., the reviews<sup>1,2</sup>). With metals as the example, it was shown that the restructuring of the quasiparticle spectrum in the superconducting transition exerts a substantial influence on the dependence of the retardation force on the dislocation velocity.<sup>2</sup> The interaction of the

dislocations with spin waves and the ensuing additional magnon retardation mechanisms of dislocations in ferromagnets were considered in Refs. 3-5.

Antiferromagnets are typical examples of crystals that are particularly rich in phase transitions, which have been well investigated both experimentally and theoretically.<sup>6</sup> The spin-wave spectra in antiferromagnets are also highly diverse, so that interest attaches to an investigation of the interaction of magnons with dislocations<sup>7</sup> and of the influence of the ground state on the retardation force.

The present paper is devoted to a theoretical study of the influence of magnons on the mobility of dislocations in antiferromagnets. It is shown that dislocation motion with even constant velocity leads to a coherent magnon emission if the dislocation velocity  $v$  exceeds the