Spin-wave theory of orientational phase transitions in RCo$_5$ compounds

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A microscopic theory is proposed for orientational phase transitions in systems consisting of two magnetic sublattices. One sublattice is magnetically ordered, while the magnetic moments of the second (paramagnetic) interact only with the magnetic moments of the first. Two physical mechanisms of the orientational phase transition are considered: the anisotropy of the interaction between the sublattices and the crystallographic anisotropy. The temperature spectrum of the spin waves above the reorientation temperature is found and contains a soft magnetic mode in the vicinity of the phase transitions. The equation of state and the threshold conditions are obtained for the start and the end of the reorientation.

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1. INTRODUCTION

The existing theory of orientational phase transitions (OPT) are either based on a phenomenological expansion of the thermodynamic potential,[1] or on the use of the molecular-field approximation.[1-3] The first approach, naturally, does not deal with the identification of the interactions in the crystal that are responsible for the reorientation of the magnetization or of the nature of the temperature dependence of the anisotropy constants. The molecular-field approximation does not make it possible to examine the dynamics of the OPT.

We consider here OPT in systems consisting of two magnetic sublattices, using quantum field theory methods. One sublattice is magnetically ordered, while the magnetic moments of the other sublattice are coupled only to the magnetic moments of the first. The interaction between the moments of the disordered sublattice are assumed to be negligibly small. The magnetically ordered sublattice will hereafter be referred to as the main one, and the other as the paramagnetic one. From these points of view, we consider in this paper OPT in compounds of a rare earth with metals of the transition group, for example in the intermetallies R_nCo_m or R_nFe_m. The magnetization reorientation will be governed by the competition between the crystallographic anisotropies of the main and paramagnetic sublattices with the anisotropy of the exchange interaction between the sublattices.

We assume furthermore that the temperature of the orientational transition is much lower than the temperature of the magnetic ordering of the crystal

$$kT \ll I, \tag{1}$$

where I is the exchange interaction between the magnetic moments of the main sublattice. This condition simplifies the problem radically, since the magnetically ordered sublattice can be represented in the form of non-interacting spin waves. We arrive thus at a paramagnetic subsystem coupled with a boson field, a subsystem whose thermodynamics and dynamics have been investigated in detail.[4,5] We can accordingly expect in our problem that when a threshold condition is satisfied there exists in the system a phase transition that leads to Bose condensation of the magnons, meaning a spontaneous rotation of the magnetization of the main sublattice. The dynamic singularities of the phase transitions should manifest themselves in the spin-wave spectrum as a soft mode and as a Goldstone mode below the transition temperature.

2. THE EQUATION OF STATE

The Holstein-Primakoff transformation

$$\begin{aligned} S_i^z&=-S+b_i^+b_i,\\ S_i^+&=(2S)^{1/2}(1-b_i^+b_i/2S)^{1/2}b_i^+,\\ S_i^-&=(2S)^{1/2}b_i(1-b_i^+b_i/2S)^{1/2}, \end{aligned} \tag{2}$$

customarily used to effect the change from spin operators to spin-wave creation and annihilation operators call for an indication of the ground state of the magnetically ordered system, i.e., an indication of the magnetization direction in the main sublattice. Consequently, before representing the magnetically ordered sublattice in terms of spin waves, it is necessary to examine the thermodynamic stability of the ground state in the crystal.

In compounds of transition and rare-earth metals, it is reasonable to regard the rare-earth ions as a paramagnetic subsystem interacting with a magnetically ordered transition-ion sublattice. We shall take into account here the following interactions that influence the OPT: 1) one-ion anisotropy of the main sublattice; 2) crystallographic one-ion first-order anisotropy of the rare-earth ions; 3) anisotropy of the exchange interaction between the transition and rare-earth ions. The first two interactions were considered in the molecular-field approximation[2,3] for RCo$_5$ compounds. Allowance for the anisotropy of the exchange interaction between the sublattices seems natural, because of the strong spin-orbit interaction in the f shell

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of the rare-earth ions.[1,5,7]

On the other hand, we disregard in this paper the following: 1) the antisymmetry of the exchange interaction between the sublattices; 2) the anisotropy of the exchange interaction between transition ions; 3) the crystallographic anisotropy of second order and higher in both sublattices; 4) exchange interaction between the rare-earth ions; 5) dipole-dipole interaction between the ions of the sublattices, and 6) the influence of the phonons on the OPT. By the same token, we disregard here the possible magnetostriction anomalies in the vicinity of the OPT. Inclusion of these relations in the theory considered below does not entail any fundamental difficulty.

Taking the foregoing into account, we express the Hamiltonian of the intermetallide in the form

$$H=-\sum_{ii'} I_{ii'}\mathbf{S}_i\mathbf{S}_{i'}-\sum_{ij}\sum_{\alpha} I_{ij}^{\alpha}S_i^{\alpha}J_j^{\alpha}+D_R\sum_{j=1}^{n}(J_j^z)^2 -D\sum_{i=1}^{N}(S_i^z)^2+|\mu|H_0\sum_{i=1}^{N}S_i^z+|\mu_R|H_0\sum_{j=1}^{n}J_j^z, \tag{3}$$

where N and n are respectively the numbers of the transition and rare-earth ions, $I_{ii'}$ is the exchange interaction between the ions of the main sublattice, I_{ij} are the anisotropic parameters of the R–Co or R–Fe exchange, D_R and D are the constants of the one-ion anisotropy of the rare earth and main (Co or Fe) sublattices, and S_i are the spin components of the Co or Fe ions. Owing to the strong spin-orbit interactions, the good quantum numbers in the rare-earth ion are the values of the total angular momentum $J=S_R+L_R$.[8]

The simplest and most lucid way of dealing the thermodynamic stability of the ground state of the model (3) is within the framework of the macroscopic description. Recognizing that the first term in the Hamiltonian (3) is rotationally invariant, we express the macroscopic invariant in the form

$$H_M=-VkM_z^2+\sum_{j=1}^{n}[A(0)M_zJ_{zj}+B(0)(M_xJ_{xj}+M_yJ_{yj})]+D_R\sum_{j=1}^{n}J_{zj}^2, \tag{4}$$

where VkM_z^2 is the anisotropy energy of the main sublattice and V is the volume of the crystal. The exchange anisotropy is taken in the simplest form

$$I_{ij}^{\alpha}=(B,B,A),\quad A(0)=\sum_r A(r),\quad B(0)=\sum_r B(r),\quad k=DN/V,$$

the value of $g\mu_B$ is set equal to unity, and the classical components $J_{\alpha j}$ and M_α are assumed.

Allowance for the excited state of the main sublattice, which are described by gradient terms, will be made in §3. As shown by Belov *et al.*,[1] the contribution of the orientational fluctuations to the thermodynamic potential of the system is small.

The stable directions of the magnetization of the main sublattice will be determined from the condition that the thermodynamic potential be a minimum. The partition function of the model (4) in a spherical coordinate system, with allowance for the constancy of the magnetization of the main sublattice in the considered temperature region (1), is of the form[5]

$$Z=\int d\Phi\sin\theta\, d\theta\exp(\beta VkM^2\cos^2\theta)Q^n(\theta,\Phi), \tag{5}$$

$$Q(\theta,\Phi)=\int d\varphi\, d\cos\alpha\exp[-\beta(D_RJ^2\cos^2\alpha+AMJ\cos\theta\cos\alpha +BMJ\sin\theta\sin\alpha\cos(\varphi-\Phi))]=4\pi^2\int_0^1 dx\exp(-\beta D_RJ^2x^2)\,\mathrm{ch}(\beta AMJx\cos\theta) \times I_0(\beta BMJ(1-x^2)^{1/2}\sin\theta), \tag{6}$$

where $I_0(x)$ is a modified Bessel function.

We confine ourselves here to the case $\beta D_RJ_2\ll 1$. Expanding $\exp(-\beta D_RJ^2x^2)$ in a series and retaining only the terms linear in D_R, we obtain[9]

$$Q(\beta,M_z)=\exp(-\beta D_RJ^2)\frac{\mathrm{sh}(a^2+b^2)^{1/2}}{(a^2+b^2)^{1/2}}\left\{1 +\beta D_RJ^2\left[\frac{a^2}{a^2+b^2}+\frac{2b^2-a^2}{(a^2+b^2)^{3/2}}L((a^2+b^2))^{1/2}\right]\right\}, \tag{7}$$
$$a=\beta BJ(M^2-M_z^2)^{1/2},\qquad b=\beta AJM_z,$$

where L is the Langevin function. The integral (5) takes the form

$$Z=G\int_{-M}^{M}dM_z\exp[\beta VkM_z^2+n\ln Q(\beta,M_z)]. \tag{8}$$

The integral in (8) can be exactly calculated in the limit as $n\to\infty$ and at constant n/V by the saddle-point method. This yields the equation of state for M_z:

$$2D\frac{B^2}{A^2}\frac{N}{n}M^2-2D_R\frac{J^2}{y^4}=\frac{L(\beta BMJy)}{y}\left[\left(\frac{B^2}{A^2}-1\right)BMJ-\frac{6D_RJ}{\beta BMy^4}\right], \tag{9}$$
$$y=\left[1-\left(1-\frac{A^2}{B^2}\right)\frac{M_z^2}{M^2}\right]^{1/2}.$$

Before we analyze this equation of state, however, it is meaningful to consider the case of isotropic exchange, $A=B$, for which the equation of state is

$$M_z\left[1-\frac{E_R}{E_M}\left(1-\frac{3L(\beta AMJ)}{\beta AMJ}\right)\right]=0. \tag{10}$$

Here

$$E_R=nD_RJ^2,\quad E_M=VkM^2 \tag{11}$$

are the anistropy energies of the rare-earth and transition sublattices, respectively. It is seen from (10) that in the absence of exchange anisotropy the threshold condition for the OPT takes the form

$$E_R>E_M. \tag{12}$$

If this condition is not satisfied, the thermodynamic potential has a minimum at $M_z=M$ at all temperatures. When the threshold condition (12) is satisfied, there exists a temperature T_0, defined by the equation

$$E_R-E_M\left(1-\frac{3L(\beta_0AMJ)}{\beta_0AMJ}\right)=0, \tag{13}$$

at which the thermodynamic potential

$$F=-\alpha(T-T_0)M_z^2$$

reverses sign and the magnetization lands jumpwise in the basal plane (Fig. 1a). It is clear that so simple a behavior of the magnetization is due primarily to the fact that no account was taken from the very outset of the higher-order crystallographic anisotropies of both sublattices. Even this analysis, however, makes it possible set in correspondence the expansion of the thermodynamic potential[1]

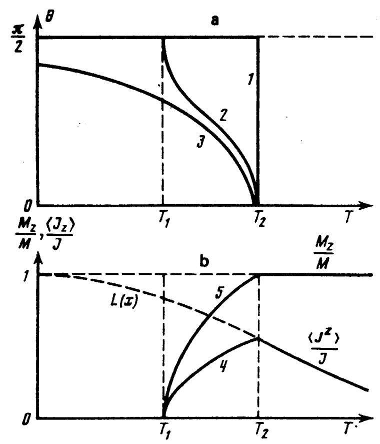


FIG. 1. Temperature dependence of the orientation of the magnetization of the main sublattice (a) and of the magnetizations M_z and $\langle J_z \rangle$ (b).

$$F=K_1(T)M_z^2+K_2(T)M_z^4 \tag{14}$$

with the constants of the microscopic Hamiltonian and obtain thus an inverse dependence of anisotropy constant K_1 on the temperature

$$K_1(T)=\beta Vk\left[\frac{E_R}{E_M}\left(1-\frac{3L(\beta AMJ)}{\beta AMJ}\right)-1\right].$$

Allowance for second-order crystallographic anisotropy in the Hamiltonian (4) adds to the thermodynamic potential (10) terms proportional to M_z^4 and makes it possible to calculate the temperature dependences of $K_2(T)$.

We proceed now to the analysis of the equation of state (9) with allowance for the exchange anisotropy, $A \neq B$. In this case, if the threshold condition

$$\frac{2B^2M^2DN/n-2A^2J^2D_R}{JBM(B^2-A^2)}<1 \tag{15}$$

is satisfied, the projection of the magnetization on the z axis of the main sublattice changes from zero to M in the temperature interval $T_1 \leqslant T \leqslant T_2$ (Fig. 1, curve 2). The variation of M_z with temperature includes then two second-order phase transitions—the beginning and the end of the reorientation. Accordingly, the temperatures of the phase transitions are determined by the equations

$$2DM^2\frac{B^2}{A^2}\frac{N}{n}-2D_RJ^2=L(\beta_1 BMJ)\left[\left(\frac{B^2}{A^2}-1\right)BMJ-\frac{6D_RJ}{\beta_1 BM}\right], \tag{16}$$

$$2DM^2\frac{A^2}{B^2}\frac{N}{n}-2D_RJ^2=L(\beta_2 AMJ)\left[\left(1-\frac{A^2}{B^2}\right)AMJ-\frac{6D_RJ}{\beta_2 AM}\right]. \tag{17}$$

Using the saddle-point method, we can obtain the temperature dependence of $\langle J_z \rangle$:

$$\langle J^z \rangle = J\frac{d}{dB}\ln Q(\beta, M_z).$$

In the approximation with $\beta D_R J^2 \ll 1$ we have expression (7) for $Q(\beta, M_z)$. The plot of the temperature dependence of $\langle J_z \rangle$ for this case is curve 4 of Fig. 1. The temperature dependence of $\langle M_z \rangle$ is shown by curve 5.

If the condition (15) is not satisfied, but the condition

$$\frac{2A^2M^2DN/n-2B^2J^2D_R}{JAM(B^2-A^2)}<1 \tag{18}$$

is, there is no phase transition at the lower temperatures, and the magnetization of the main sublattice does not reach the basal plane (Fig. 1, curve 3). A comparison of (16) and (17) shows that the existence of two successive phase transitions is due to the anisotropy of the exchange interaction between the main and paramagnetic sublattices.

The foregoing analysis, carried out within the framework of the classical description of a magnetically ordered crystal, shows that when condition (18) is satisfied there exists a temperature region $T \geqslant T_2$ in which the ground state of the entire system is determined only by the constants of the main sublattice. This result can be easily understood by recognizing that with increasing temperature the magnetization of the paramagnetic sublattice decreases and accordingly its contribution to the orientational state of the entire system decreases.

3. DYNAMICS OF HIGH TEMPERATURE PHASE

In the high temperature phase $T \geqslant T_2$ the magnetization of the main subsystem in the ground state is directed along the z axis. We can use therefore the transformation (2) in the Hamiltonian (3), and the angular momentum of the rare-earth ion can be represented in terms of the Fermi operators

$$J_j^z=\sum_{M=-J}^{J} Ma_{jM}^+a_{jM}, \quad J_j^+=\sum_{M=-J}^{J}[J(J+1)-M(M+1)]^{1/2}a_{jM+1}^{+}a_{jM},$$
$$J_j^-=\sum_{M=-J}^{J}[J(J+1)-M(M-1)]^{1/2}a_{jM-1}^{+}a_{jM}. \tag{19}$$

Taking the Fourier transforms of the Bose operators (2), we obtain

$$H=\sum_{\mathbf{k}}\omega(\mathbf{k})b_{\mathbf{k}}^+b_{\mathbf{k}}+\sum_{jM}\varepsilon_M a_{jM}^+a_{jM}$$
$$+\frac{1}{N}\sum_{j=1}^{n}\sum_{\mathbf{kq}}\sum_{M}A(\mathbf{q})Mb_{\mathbf{k}}^+b_{\mathbf{k+q}}a_{jM}^+a_{jM}\exp(i\mathbf{qr}_j)$$
$$+\left(\frac{S}{2N}\right)^{1/2}\sum_{j=1}^{n}\sum_{\mathbf{q}}\sum_{M}B(\mathbf{q})[J(J+1)-M(M+1)]^{1/2}[a_{jM+1}^{+}a_{jM}b_{\mathbf{q}}\exp(i\mathbf{qr}_j)+\text{H.c.}]; \tag{20}$$

$$\omega(\mathbf{k})=2SD+|\mu_e|H_0+\alpha\mathbf{k}^2=\Delta+|\mu_e|H_0+\alpha\mathbf{k}^2,$$
$$\varepsilon_M=(|\mu_R|H_0-A(0)S)M+D_RM^2,$$
$$A(\mathbf{q})=\sum_{\mathbf{r}}A(\mathbf{r})e^{-i\mathbf{qr}}, \quad B(\mathbf{q})=\sum_{\mathbf{r}}B(\mathbf{r})e^{-i\mathbf{qr}}. \tag{21}$$

We have left out of the Hamiltonian (20) the terms that describe scattering of spin waves by one another, since they can be neglected in the considered temperature region (1).[10]

We introduce the magnon Green's functions and the fermion Green's functions of the rare-earth angular momenta J (Ref. 11):

$$D(\mathbf{k},\omega_m)=\int_0^\beta e^{i\omega_m\tau}\langle T\{b_{\mathbf{k}}(\tau)b_{\mathbf{k}}^+(0)\}\rangle d\tau,$$
$$G_{MM'}(\mathbf{r}_j\ \omega_n)=\int_0^\beta e^{i\omega_n\tau}\langle T\{a_{jM'}(\tau)a_{jM}^+(0)\}\rangle d\tau, \tag{22}$$
$$\omega_m=2\pi mkT, \quad \omega_n=(2n+1)\pi kT, \quad m,\ n=0,\ \pm1,\ \pm2,\ldots.$$

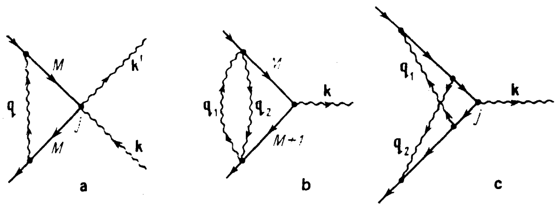
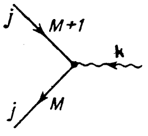


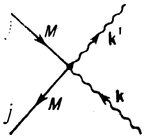
FIG. 2.

The respective Green's functions will be designated in the diagrams by wavy and straight lines.

It follows from the Hamiltonian (20) that the Feynman diagrams contain two types of bare vertex functions



$$=B(\mathbf{k})\,(S/2N)^{1/2}[J(J+1)-M(M+1)]^{1/2}\exp(i\mathbf{k}\mathbf{r}_j),$$



$$=A(\mathbf{k}-\mathbf{k}')N^{-1}M\exp[i(\mathbf{k}-\mathbf{k}')\mathbf{r}_j], \tag{23}$$

where the first diagrams describes magnon absorption by a RE ion, and the second magnon scattering by the RE angular momenta.

We determine the poles of the magnon Green's function (22), analytic continuation of which determines the transverse dynamic susceptibility of the ferromagnet.[11] We shall show first that under condition (1) it suffices to retain in the diagram equations only the bare vertex functions (23). Let us take by way of example the diagrams of Fig. 2. All these diagrams contain one or more internal magnon lines. Diagram a of Fig. 2 is equal to

$$\frac{AB^2S}{2}\frac{1}{\beta N}\sum_{\mathbf{q}m}\frac{M[J(J+1)-M(M+1)]}{i\omega_m-\omega(\mathbf{q})}\times(i\omega_n-i\omega_m-\varepsilon_M)^{-1}(i\omega_n-i\omega_m-i\omega_{m'}-\varepsilon_{M+1})^{-1}. \tag{24}$$

The sum over m in (24) converges like m^{-3} and can therefore be discarded. As for the sum over q, it is seen from (24) that the principal role is played by the term with $m=0$.

The question of estimating the vertex functions in Fig. 2(a) reduces thus to an estimate of an integral of the form

$$\frac{a^3}{\beta(2\pi)^3}\int_0^{\pi/a}\frac{d^3\mathbf{q}}{\omega(\mathbf{q})}. \tag{25}$$

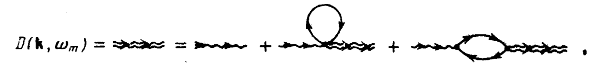
The main contribution to the integral is made by the region $0\leqslant qa\leqslant[\Delta/2SI(0)]^{1/2}$, where a is the dimension of the unit cell of the cubic crystal. Putting $\Delta\ll 2SI(0)$, we find from (21) that we can confine ourselves to a quadratic dispersion law in the spin-wave spectrum

$$\omega(\mathbf{q})=\Delta+SI(0)q^2a^2+|\mu_e|H_0. \tag{26}$$

Integrating (25) with the aid of (26) we readily find that the integral as well as the vertex function (24) are of the order of smallness $1/\beta I(0)$. The other vertex functions are similarly estimated. Summarizing these estimates, we can state that those diagrams which contain one or more internal magnon lines are small of the order $1/\beta I(0)$. We note that a like smallness parameter appears when scattering of spin waves by one another is considered.[10]

As a result, the Dyson equation for the magnon Green's function takes the form

$D(\mathbf{k},\omega_m) =$



(27)

where the fermion Green's functions coincide with the zero functions

$$G_{MM'}(r_j,\omega_n)=-\frac{\delta_{MM'}}{i\omega_n-\varepsilon_M-\mu} \tag{28}$$

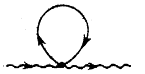
because any mass operator in a fermion Green's function has an order of smallness $1/\beta I(0)$ or higher. The parameter μ in (28) is introduced to avoid the contribution of extra states in the spin states with the aid of the projection operator[12,13]

$$P=Z_J^{-1}\lim_{\mu\to\infty}[\exp(\beta\mu)], \tag{29}$$

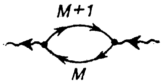
where Z_J is the partition function of the paramagnetic subsystem:

$$Z_J=\sum_M\exp(-\beta\varepsilon_M). \tag{30}$$

With the aid of (20), (22), and (28)–(30) we get



$$=(-1)AP\sum_M\frac{M}{\exp[\beta(\varepsilon_M+\mu)]+1}=-A\langle J^z\rangle, \tag{31}$$



$$=(-1)\frac{B^2S}{2}\frac{J(J+1)-M(M+1)}{i\omega_m+\varepsilon_{M+1}-\varepsilon_M}\times P\{\exp[-\beta(\varepsilon_M+\mu)]-\exp[-\beta(\varepsilon_{M+1}+\mu)]\}. \tag{32}$$

Equations (27)–(32) yield an equation for the spin-wave resonance frequencies:

$$\Omega-\omega(\mathbf{q})-A(0)\frac{n}{N}\langle J^z\rangle=\frac{B^2(\mathbf{q})S}{2}\frac{n}{N}\sum_M\frac{J(J+1)-M(M+1)}{\Omega-\varepsilon_M+\varepsilon_{M+1}}\times[\exp(-\beta\varepsilon_M)-\exp(-\beta\varepsilon_{M+1})]\Big[\sum_M\exp(-\beta\varepsilon_M)\Big]^{-1}, \tag{33}$$

$$\langle J^z\rangle=\sum_M M\exp(-\beta\varepsilon_M)\Big/\sum_M\exp(-\beta\varepsilon_M).$$

Equation (33) has in the general case $2J+1$ roots, constituting in Fig. 3 the points of intersection of the straight line and the curves. The dashed verticals mark the zeros of the denominator in the right-hand side of (33), equal according to (21) to

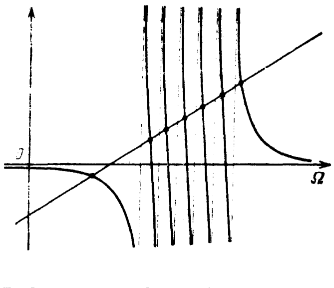


FIG. 3. Graphic solution of the equation for the resonant frequencies of an intermetallide.

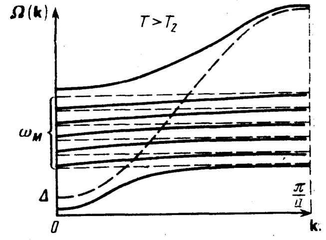


FIG. 4. Dispersion spectrum of collective oscillations in an intermetallide.

$$\omega_M = A(0)S - |\mu_R| H_0 - (2M+1)D_R. \tag{34}$$

The oblique straight line is the left-hand side of (33) at $\mathbf{q}=0$. As seen from Fig. 3, it is possible to choose directly $2J-1$ solutions, represented by the points located between the dashed verticals and having weak dispersion and temperature dependences (Figs. 4, 5). There exists one solution represented in Fig. 3 by point on the extreme right, with strong temperature and dispersion dependences, but not exhibiting a critical behavior (hard mode). Finally, the solution on the extreme left is critical (soft mode). The appearance of a null solution leads to thermodynamic instability in the system considered. It is seen already from Fig. 3 and Eq. (34) that the instability can set in when the temperature is lowered both because of the crystallographic anisotropy of the "easy plane" of the "easy plane" type in the system, and on account of the anisotropy of the exchange between the sublattices.

We obtain the temperature T_2 of the orientational phase transition assuming the crystallographic anisotropy to be small compared with the exchange between the sublattices

$$JD_R \ll A(0)S.$$

Expanding the denominator in the right-hand side of (33):

$$\frac{1}{\Omega-\varepsilon_M+\varepsilon_{M+1}} \approx \frac{1}{\Omega-E_0} - \frac{D_R(2M+1)}{(\Omega-E_0)^2},$$

where $E_0 = A(0)S - |\mu R| H_0$, and using the commutation relations for the operators J^z, J^+, and J^-, we obtain

$$\begin{gathered}\sum_{M=-J}^{J-1} [J(J+1)-M(M+1)][\exp(-\beta\varepsilon_M) \\ - \exp(-\beta\varepsilon_{M+1})] \Big/ \sum_M \exp(-\beta\varepsilon_M) = -2\langle J^z\rangle, \\ \sum_{M=-J}^{J-1} [J(J+1)-M(M+1)](2M+1)[\exp(-\beta\varepsilon_M) \\ - \exp(-\beta\varepsilon_{M+1})] \Big/ \sum_M \exp(-\beta\varepsilon_M) = 2[J(J+1)-3\langle (J^z)^2\rangle].\end{gathered} \tag{35}$$

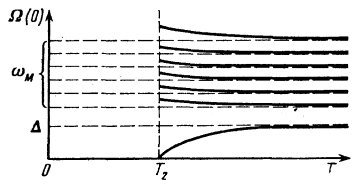


FIG. 5. Temperature dependence of homogenous oscillations in an intermetallide.

Equation (33) for the spin-wave resonance frequencies takes therefore the form

$$\Omega-\omega(\mathbf{q}) - A(0)\frac{n}{N}\langle J^z\rangle - B^2(\mathbf{q})S\frac{n}{N}\left\{\frac{\langle J^z\rangle}{\Omega-E_0} + \frac{D_R[J(J+1)-3\langle (J^z)^2\rangle]}{(\Omega-E_0)^2}\right\} = 0. \tag{36}$$

We put $D_R=0$ in (36). The equation for the phase-transition temperature T_2 then takes the form

$$JB_J[\beta_2(A(0)S-|\mu_R|H_0)] = \frac{N}{n}\frac{A(0)(2SD+|\mu|H_0)}{B^2(0)-A^2(0)}$$

where $B_J(x)$ is a Brillouin function. In the general case, at $D_R \neq 0$, the equation for the temperature T_2 of the OPT is

$$\begin{gathered}\frac{N}{n}A(0)(2SD+|\mu|H_0) = (B^2(0)-A^2(0))\langle J^z\rangle|_{\beta=\beta_2} \\ - \frac{D_R B^2(0)}{A(0)S}[J(J+1)-3\langle (J^z)^2\rangle]|_{\beta=\beta_2}.\end{gathered} \tag{37}$$

It is easy to change from this equation to (17) by recognizing that at $J \gg 1$

$$\langle (J^z)^2\rangle = J^2\left(1-\frac{2L(x)}{x}\right),$$

where $x=\beta A(0)SJ$. At $A=B$ we obtain Eq. (10). Thus, the existence of a soft mode is a characteristic of an OPT of either first or second order.

In the case of the experimentally investigated $\mathrm{RCo_5}$ compounds,[2,14,15] the quantity $\beta D_R J^2$ is comparable with unity in the vicinity of the OPT temperature. Therefore the temperature behavior of the magnetization $\langle J_z\rangle$ of the rare-earth sublattice will differ noticeably from a Brillouin behavior,[14] as is seen from (21) and (35).

4. COMPARISON WITH EXPERIMENT

We did not consider in §2 the magnetization of the rare-earth sublattice at $\beta D_R J^2 \sim 1$. Equation (37) allows us to fill this gap and compare the results with the experimental data not only on the temperature dependence of the magnetization orientation of the entire system, but also on its value at the point T_2.

For a comparison of the results with experiment, we have chosen the well-investigated compound $Dy\mathrm{Co_5}$. The total angular momentum of the Dy^{3+} ions is $J=15/2$; the one-ion anisotropy energy of the Co ions is $D_M S^2 = 35$ K/atom,[2] and the magnetic moment of the Co sublattice per formula unit is $5M = 7.7\mu_B$.[15] Recognizing that the total magnetic moment per $Dy\mathrm{Co_5}$ cell as $T\to 0$ is $\approx 1.1\mu_B$;[2] we obtain for the moment of the Dy^{3+} ions $m \approx 8.8\ \mu_B$. The transverse exchange between sublattices can be estimated from measurements of the temperature at which the total magnetization of the ferrimagnet vanishes (the compensation temperature) $T_c = 125\,K$ (Ref. 15) under the assumption that the magnetization of the rare-earth sublattice at this temperature is close to the Langevin function, which yields $BM = 133.3\,K$. The parameters B/A and D_R are obtained from the equations at the temperatures of the start and end of the reorientation [Eqs. (16) and (17)] in $Dy\mathrm{Co_5}$ in the case when the external magnetic field is turned off. Substituting $T_1 \approx 310\,K$ in (16) and $T_2 \approx 360\,K$ in (17) we obtain

$$B/A=1.0676, \quad D_R=7.5\ \mathrm{K}. \tag{38}$$

Knowing now all the parameters of the spin Hamiltonian (3), it is easy to determine the temperature dependence of the angle between the magnetization of the main sublattice and the c axis.

The last stage in the comparison of the theory with experiment is the substitution of the obtained values of (38) in Eq. (37), which enables us to find $\langle J_z \rangle$ at $\beta=\beta_2$. We use here the approximate equality

$$\langle (J^z)^2 \rangle \approx J(J+1)/3+\langle J^z \rangle^2,$$

which is valid in the considered temperature region. We obtain ultimately

$$\langle J^z \rangle_{\beta=\beta_2} \approx 3.63.$$

Recognizing that $\langle J^z \rangle \to 15/2$ as $T \to 0$ (this corresponds to a magnetic moment $m=8.8\ \mu_B$), we obtain the magnetic moment of the ion at $T=T_2$:

$$\langle m \rangle_{\beta=\beta_2} \approx 4.26 \mu_B,$$

which yields the total magnetic moment per formula unit at $T=T_2$:

$$5M-\langle m \rangle_{\beta=\beta_2} \approx 3.44 \mu_B.$$

This result agrees with experiment[2] with good accuracy and indicates that allowance for the anisotropy of the exchange interaction between the ions of the transition and rare-earth groups is important for the analysis of the OPT.

5. DISCUSSION

We did not consider the influence of an external magnetic field on the OPT parameters. It follows from (37) at first glance that the OPT temperature can be raised by directing the external magnetic field H_0 opposite to the z axis and by the same token decrease the gap in the spin-wave spectrum. In this case, however, the ground state of the magnetically ordered sublattice, in which all the electron spins were directed downward (the magnetic moments, upward) become unstable, since the state with lowest energy is realized already for the up-directed electron spins.[2] This type of problem pertains to an OPT induced by an external magnetic field, is outside the scope of equilibrium thermodynamics, and can be solved by the methods of Tomita and Murakami as well as of Patashinskiĭ and Shumilo.[16-18]

The fact that the analysis of the orientational phase transition with the aid of the bare vertex functions (23) of the diagram expansion is correct within the framework of condition (1) indicates that the condition (1) is the criterion for the applicability of the approximation of the mean-field theory. The physical reason is that in the absence of magnon scattering by one another the effective radius of the interaction via the spin waves is limited only by the dimensions of the crystal, i.e., the interaction is long-range.

It is easy to transfer the approach developed in the present paper to magnetically ordered systems, in which the orientational phase transition is due to the anisotropic interaction of the electron and nuclear spins.[19]

It must be emphasized that research into the dynamics of the intermetallides R_nCo_m and R_nFe_m can yield valuable additional information on the thermodynamic parameters of the system. As seen from Figs. 4 and 5, it is possible to determine directly the angular momentum of a rare-earth ion, the transition temperature the anisotropy constants of both sublattices, and the magnitude of the exchange between the sublattices.

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