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TEMPERATURE-DEPENDENT MAGNON ENERGIES IN Cr_2O_3

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Two formulae for temperature dependent magnon energies in Cr_2O_3 are obtained using the method of Bloch and the method of Nagai. The connection between them is discussed. Comparison of the numerical results with the experimental data of Samuelsen shows disagreement for higher temperatures.

1. *Introduction*

Different methods are used to obtain theoretically the temperature dependent magnon energies. One of them is based on the Oguchi [1] expansion and the minimum property of the free energy (Peierls [2]). This method was first introduced by Bloch [3] for cubic ferromagnet and antiferromagnet with one interaction constant. In this paper the same method will be used to obtain the temperature dependent magnon energies in Cr_2O_3. The final formula will be given in the form of an implicit equation which must be solved selfconsistently. Then the same effect will be described by the approximation first introduced for antiferromagnets by Nagai [4], and the connection between the two methods will be discussed. Finally, we shall compare the numerical results based on these theories with the experimental results of Samuelsen [5], [6].

2. *The Hamiltonian and its transformations*

The Hamiltonian for Cr_2O_3 will be assumed in the following form:

$$\mathscr{H} = -G\sum_{l} S_l^z + G\sum_{m} S_m^z - \sum_{l\neq l'} J_{ll'}\boldsymbol{S}_l\cdot\boldsymbol{S}_{l'} - \sum_{m\neq m'} J_{mm'}\boldsymbol{S}_m\cdot\boldsymbol{S}_{m'} - 2\sum_{lm} J_{lm}\boldsymbol{S}_l\cdot\boldsymbol{S}_m \tag{1}$$

(in the first two double summations each interaction is taken twice).

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G is the effective anisotropy constant, $J_{ll'}$ are the interaction constants between spins in the first sublattice, $J_{mm'}$ are the interaction constants between spins in the second sublattice, and J_{lm} are the interaction constants between spins in the first and in the second sublattice. Cr_2O_3 has the corrundum ($\alpha-Al_2O_3$) crystal structure, it is an antiferromagnet with $T_N = 308°K$. The crystal and magnetic structure are discussed elsewhere [6, 7]. We shall restrict ourselves to five interaction constants, which according to Samuelsen *et al.* [6]

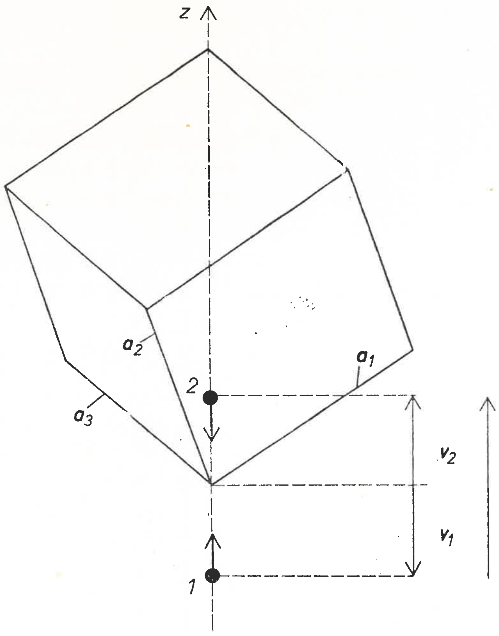

Fig. 1. Small unit cell of Cr_2O_3. z-axis along the three-fold symmetry axis, $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ — the primitive lattice vectors, $\mathbf{v}_1$, $\mathbf{v}_2$ — position vectors of Cr ions, $\mathbf{v} = \mathbf{v}_2 - \mathbf{v}_1$

will be called J_1, J_2, J_3, J_4, J_5. We assume as the unit cell the so-called small unit cell to which two Cr ions belong with their spins directed parallel to the z-axis in the case of Cr ion number "1" and antiparallel in the case of Cr ion number "2" (see Fig. 1.)

Below, in Table I, we give the number of neighbours with particular interaction constant and their position vectors.

Now, using the Oguchi expansion, we shall perform two kinds of transformations of the Hamiltonian (1).

Transformation I: $S_l \to a_l, a_l^\dagger$; $S_m \to b_m, b_m^\dagger$

$$S_l^+ = \sqrt{2S}\, f_l a_l, \quad S_l^- = \sqrt{2S}\, a_l^\dagger f_l, \quad S_l^z = S - a_l^\dagger a_l, \quad f_l \cong 1 - a_l^\dagger a_l/4S$$

$$S_m^+ = \sqrt{2S}\, b_m^\dagger f_m, \quad S_m^- = \sqrt{2S}\, f_m b_m, \quad S_m^z = -S + b_m^\dagger b_m, \quad f_m \cong 1 - b_m^\dagger b_m/4S \quad (2)$$

a_l, b_m fulfil the usual Bose commutation relations.

TABLE I

	Number of neighbours	Interaction constant	Position vectors of the neighbours
Cr ion "1"	1	J_1	$\boldsymbol{v}_2$
	3	J_2	$-\boldsymbol{a}_1+\boldsymbol{v}_2,\ -\boldsymbol{a}_2+\boldsymbol{v}_2,\ -\boldsymbol{a}_3+\boldsymbol{v}_2$
	3	J_3	$-\boldsymbol{a}_1-\boldsymbol{a}_2+\boldsymbol{v}_2,\ -\boldsymbol{a}_1-\boldsymbol{a}_3+\boldsymbol{v}_2,\ -\boldsymbol{a}_2-\boldsymbol{a}_3+\boldsymbol{v}_2$
	6	J_4	$\pm\boldsymbol{a}_1+\boldsymbol{v}_1,\ \pm\boldsymbol{a}_2+\boldsymbol{v}_1,\ \pm\boldsymbol{a}_3+\boldsymbol{v}_1$
	1	J_5	$-\boldsymbol{a}_1-\boldsymbol{a}_2-\boldsymbol{a}_3+\boldsymbol{v}_2$
Cr ion "2"	1	J_1	$\boldsymbol{v}_1$
	3	J_2	$\boldsymbol{a}_1+\boldsymbol{v}_1,\ \boldsymbol{a}_2+\boldsymbol{v}_1,\ \boldsymbol{a}_3+\boldsymbol{v}_1$
	3	J_3	$\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{v}_1,\ \boldsymbol{a}_1+\boldsymbol{a}_3+\boldsymbol{v}_1,\ \boldsymbol{a}_2+\boldsymbol{a}_3+\boldsymbol{v}_1$
	6	J_4	$\pm\boldsymbol{a}_1+\boldsymbol{v}_2,\ \pm\boldsymbol{a}_2+\boldsymbol{v}_2,\ \pm\boldsymbol{a}_3+\boldsymbol{v}_2$
	1	J_5	$\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3+\boldsymbol{v}_1$

Transformation II: $a_l^\dagger, a_l \to a_k^\dagger, a_k;\ b_m^\dagger, b_m \to b_k^\dagger, b_k$

$$a_l^\dagger = (1/\sqrt{N_0}) \sum_k a_k^\dagger \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_l), \qquad a_l = (1/\sqrt{N_0}) \sum_k a_k \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_l)$$

$$b_m^\dagger = (1/\sqrt{N_0}) \sum_k b_k^\dagger \exp(-i\boldsymbol{k}\cdot\boldsymbol{r}_m), \qquad b_m = (1/\sqrt{N_0}) \sum_k b_k \exp(i\boldsymbol{k}\cdot\boldsymbol{r}_m). \tag{3}$$

The new operators $a_k, a_k^\dagger, b_k, b_k^\dagger$ again fulfil the Bose commutation relations. Summation runs over $\boldsymbol{k}$, in the first Brillouin zone, $\boldsymbol{r}_l$, $\boldsymbol{r}_m$ are the position vectors of the spins $\boldsymbol{S}_l$ and $\boldsymbol{S}_m$ respectively, N_0 is the number of lattice points in one sublattice.

The Hamiltonian (1) after performing the first and the second transformation has the following form:

$$\underset{}{\mathscr{H}} = \underset{\text{constant term}}{\mathscr{H}_{\text{II}}^{(0)}} + \underset{\text{bilinear terms}}{\mathscr{H}_{\text{II}}^{(1)}} + \underset{\text{biquadratic terms}}{\mathscr{H}_{\text{II}}^{(2)}} \tag{4}$$

$$\mathscr{H}_{\text{II}}^{(0)} = -2SN_0G+2S^2N_0(\eta-\tilde{\eta}). \tag{4a}$$

$$\mathscr{H}_{\text{II}}^{(1)} = \sum_k (-2S\eta+G+2S\tilde{\eta}(1-\zeta_k))\,(a_k^\dagger a_k+b_k^\dagger b_k)+$$

$$+[\sum_k(-2S\eta\gamma_k)a_kb_k+\text{h.c.}]. \tag{4b}$$

$$\mathscr{H}_{\text{II}}^{(2)} = (\eta/2N_0)\,[\sum_{\{k\}}(a_1^\dagger a_2a_3b_4+b_1^\dagger b_2b_3a_4)\gamma_4\delta(\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3+\boldsymbol{k}_4)+\text{h.c.}]+$$

$$+(2\eta/N_0)\sum_{\{k\}}(a_1^\dagger a_2b_3^\dagger b_4)\gamma_{4-3}\delta(\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3+\boldsymbol{k}_4)+$$

$$+(\tilde{\eta}/2N_0)\,[\sum_{\{k\}}(a_1^\dagger a_2^\dagger a_3a_4+b_1^\dagger b_2^\dagger b_3b_4)\zeta_4\delta(\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3-\boldsymbol{k}_4)+\text{h.c.}]-$$

$$-(\tilde{\eta}/N_0)\sum_{\{k\}}(a_1^\dagger a_2a_3^\dagger a_4+b_1^\dagger b_2b_3^\dagger b_4)\zeta_{3-4}\delta(\boldsymbol{k}_1-\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{k}_4). \tag{4c}$$

Here $\{\boldsymbol{k}\}$ means $\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3, \boldsymbol{k}_4, a_1$ stands instead of a_{k_1} *etc.*

$$\eta = J_1+3J_2+3J_3+J_5 \qquad (\eta < 0 \text{ for } Cr_2O_3)$$

$$\tilde{\eta} = 6J_4;\ \zeta_k = (\cos(\boldsymbol{k}\cdot\boldsymbol{a}_1)+\cos(\boldsymbol{k}\cdot\boldsymbol{a}_2)+\cos(\boldsymbol{k}\cdot\boldsymbol{a}_3))/3$$

$$\gamma_k = \exp(i\boldsymbol{k}\cdot\boldsymbol{v})\{j_1+j_2[\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_1)+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_2)+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_3)]+$$
$$+j_3[\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_2))+\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_3))+\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_2+\boldsymbol{a}_3))]+$$
$$+j_5\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3))\} = \gamma_k(j_1j_2j_3j_5)$$

where

$$j_i = J_i/\eta \qquad (i = 1\ldots 5); \qquad j_1+3j_2+3j_3+j_5 = 1. \tag{4d}$$

Introducing the symbols: $\alpha = G/(-2S\eta)$,

$$\mathscr{A}_k = (-2S\eta)A_k,\ A_k = 1+\alpha-6j_4(1-\zeta_k),$$
$$\mathscr{B}_k = (-2S\eta)\gamma_k \tag{4e}$$

we can write the bilinear part (4b) in the form:

$$\mathscr{H}_{\mathrm{II}}^{(1)} = \sum_k \mathscr{A}_k(a_k^\dagger a_k+b_k^\dagger b_k)+\mathscr{B}_k a_k b_k+\mathscr{B}_k^* a_k^\dagger b_k^\dagger. \tag{4f}$$

3. *The method of Bloch applied to* Cr_2O_3

In order to apply this method for the case of Cr_2O_3 we have to perform a new transformation in such a way that $\mathscr{H}_{\mathrm{II}}^{(1)}$ will become diagonal.

Transformation III: $a_k^\dagger, a_k, b_k^\dagger, b_k \rightarrow \alpha_k^\dagger, \alpha_k, \beta_k^\dagger, \beta_k$

$$a_k^\dagger = l_k^{(1)}\alpha_k^\dagger + l_k^{(2)}\beta_k, \qquad b_k^\dagger = l_k^{(2)}\alpha_k + l_k^{(1)}\beta_k^\dagger$$
$$a_k = l_k^{(1)*}\alpha_k + l_k^{(2)*}\beta_k^\dagger, \qquad b_k = l_k^{(2)*}\alpha_k^\dagger + l_k^{(1)*}\beta_k. \tag{5}$$
$$l_k^{(1)} = [(\mathscr{A}_k+\varepsilon_k^{(0)})/2\varepsilon_k^{(0)}]^{1/2}\exp(i\varphi_k/2)$$
$$l_k^{(2)} = -[(\mathscr{A}_k-\varepsilon_k^{(0)})/2\varepsilon_k^{(0)}]^{1/2}\exp(i\varphi_k/2)$$
$$\exp(i\varphi_k) = \mathscr{B}_k/|\mathscr{B}_k|; \qquad |l_k^{(1)}|^2-|l_k^{(2)}|^2 = 1$$

$$\varepsilon_k^{(0)} = (\mathscr{A}_k^2-|\mathscr{B}_k|^2)^{1/2} = (-2S\eta)(A_k^2-|\gamma_k|^2)^{1/2} \overset{\mathrm{df}}{=} (-2S\eta)E_k. \tag{5a}$$

The new operators $\alpha_k^\dagger, \alpha_k, \beta_k^\dagger, \beta_k$ fulfil again the Bose commutation relations.

$\mathscr{H}_{\mathrm{II}}^{(1)}$ transformed in this way contributes to the constant term the expression

$$\delta\mathscr{H}_{\mathrm{III}}^{(0)} = \sum_k(\varepsilon_k^{(0)}-\mathscr{A}_k) = (-2S\eta)\sum_k(E_k-A_k) \tag{5b}$$

and gives besides:

$$\sum_k \varepsilon_k^{(0)}(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) = \sum_k \varepsilon_k^{(0)}(n_k + n_k'). \tag{5c}$$

We have introduced here the usual notation:

$$\alpha_k^\dagger \alpha_k = n_k, \quad \beta_k^\dagger \beta_k = n_k'.$$

From the transformed $\mathscr{H}_{\mathrm{II}}^{(2)}$ we take only contributions to the diagonal terms, *i.e.* to the constant term and to the terms proportional to: $n_k, n_k', n_{k_1}n_{k_2}, n_{k_1}'n_{k_2}', n_{k_1}n_{k_2}'$. From each biquadratic term in $\mathscr{H}_{\mathrm{II}}^{(2)}$ we get 16 products of 4 new operators. For instance, from $a_{k_1}^\dagger a_{k_2} a_{k_3} b_{k_4}$ we get 16 terms. As an example let us consider one of them which is proportional to

$$\sum_{\{k\}} \beta_{k_1}\alpha_{k_2}\beta_{k_3}^\dagger \alpha_{k_4}^\dagger \delta(\boldsymbol{k}_1 - \boldsymbol{k}_2 - \boldsymbol{k}_3 + \boldsymbol{k}_4)\gamma_{k4} l_{k_1}^{(2)} l_{k_2}^{(1)*} l_{k_3}^{(2)*} l_{k_4}^{(2)*}.$$

Here, from all possible $\boldsymbol{k}$ vectors we take only those which fulfil the relation $\boldsymbol{k}_1 = \boldsymbol{k}_3$, $\boldsymbol{k}_2 = \boldsymbol{k}_4$, so that we consider only:

$$\beta_{k_1}\beta_{k_1}^\dagger \alpha_{k_2}\alpha_{k_2}^\dagger = 1 + \beta_{k_1}^\dagger \beta_{k_1} + \alpha_{k_2}^\dagger \alpha_{k_2} + \beta_{k_1}^\dagger \beta_{k_1} \alpha_{k_2}^\dagger \alpha_{k_2}.$$

In this way we obtain contributions to the constant term: $\delta\mathscr{H}_{\mathrm{III}'}^{(0)}$, to the bilinear terms: $\sum_k \delta\varepsilon_k^{(0)}(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k)$, and to the biquadratic terms.

The approximate Hamiltonian obtained after the third transformation has the following final form:

$$\mathscr{H} \cong \mathscr{H}_{\mathrm{II}}^{(0)} + \delta\mathscr{H}_{\mathrm{III}}^{(0)} + \delta\mathscr{H}_{\mathrm{III}'}^{(0)} + \sum_k (\varepsilon_k^{(0)} + \delta\varepsilon_k^{(0)})(n_k + n_k') +$$
$$+ \sum_{k_1k_2} B_{k_1k_2}^{(1)}(n_{k_1}n_{k_2} + n_{k_1}'n_{k_2}') + \sum_{k_1k_2} B_{k_1k_2}^{(2)} n_{k_1}n_{k_2}' \tag{6}$$

where

$$\delta\mathscr{H}_{\mathrm{III}'}^{(0)} = (\eta/2N_0)\{[\sum_q (A_q - E_q)/E_q]^2 + \sum_{q_1q_2} (\gamma_{q_1}\gamma_{q_2}^*\gamma_{q_2-q_1})/E_{q_1}E_{q_2} -$$
$$-2[\sum_q (A_q - E_q)/E_q][\sum_q |\gamma_q|^2/E_q]\} +$$
$$+(\tilde{\eta}/2N_0)[\sum_q (A_q - E_q)(1-\zeta_q)/E_q]^2. \tag{6a}$$

$$\varepsilon_k^{(0)} + \delta\varepsilon_k^{(0)} = \varepsilon_k^{(0)}(1 + c_k/2S) \stackrel{\mathrm{df}}{=} \varepsilon_k; \quad c_k = c_k^{(1)} + c_k^{(2)} + c_k^{(3)}$$
$$c_k^{(1)} = [(A_k - |\gamma_k|^2)/E_k^2](1/N_0)\sum_q [1 - (A_q - |\gamma_q|^2)/E_q]$$
$$c_k^{(2)} = (|\gamma_k|^2/E_k^2)(1/N_0)\sum_q (|\gamma_q|^2/E_q) - \mathrm{Re}\,[(\gamma_k/E_k^2)(1/N_0)\sum_q \gamma_q^*\gamma_{q-k}/E_q]$$
$$c_k^{(3)} = (\tilde{\eta}/\eta)(A_k(1-\zeta_k)/E_k^2)(1/N_0)\sum_q [A_q(1-\zeta_q)/E_q - 1]. \tag{6b}$$

$$B^{(1)}_{k_1k_2} = (\eta/2N_0)\,[(A_{k_1}A_{k_2}-A_{k_1}|\gamma_{k_2}|^2-A_{k_2}|\gamma_{k_1}|^2+\gamma_{k_1}\gamma^*_{k_2}\gamma_{k_2-k_1})/E_{k_1}E_{k_2}-1]+$$
$$+(\tilde{\eta}/2N_0)\,[A_{k_1}A_{k_2}/E_{k_1}E_{k_2}+1]\,[\zeta_{k_1}+\zeta_{k_2}-\zeta_{k_1-k_2}-1] \tag{6c}$$
$$B^{(2)}_{k_1k_2} = (\eta/N_0)\,[(A_{k_1}A_{k_2}-A_{k_1}|\gamma_{k_2}|^2-A_{k_2}|\gamma_{k_1}|^2+\mathrm{Re}\,\gamma_{k_1}\gamma^*_{k_2}\gamma_{k_2-k_1})/E_{k_1}E_{k_2}+1]+$$
$$+(\tilde{\eta}/N_0)\,[A_{k_1}A_{k_2}/E_{k_1}E_{k_2}-1]\,[\zeta_{k_1}+\zeta_{k_2}-\zeta_{k_1-k_2}-1]. \tag{6d}$$

Now, according to the method of Bloch [3], we write the approximate temperature dependent free energy F in the form:

$$F = \text{const.}+\sum_k \varepsilon_k(\langle n_k\rangle+\langle n'_k\rangle)+\sum_{k_1k_2} B^{(1)}_{k_1k_2}\langle n_{k_1}\rangle\,\langle n_{k_2}\rangle+$$
$$+\sum_{k_1k_2} B^{(1)}_{k_1k_2}\langle n'_{k_1}\rangle\,\langle n'_{k_2}\rangle+\sum_{k_1k_2} B^{(2)}_{k_1k_2}\langle n_{k_1}\rangle\,\langle n'_{k_2}\rangle+$$
$$+k_BT[\sum_k \langle n_k\rangle \ln\langle n_k\rangle-\sum_k(\langle n_k\rangle+1)\ln(\langle n_k\rangle+1)+$$
$$+\sum_k \langle n'_k\rangle \ln\langle n'_k\rangle-\sum_k(\langle n'_k\rangle+1)\ln(\langle n'_k\rangle+1)]. \tag{7}$$

Putting

$$\langle n_k\rangle = \langle n'_k\rangle = 1/(\exp(\varepsilon_k(T)/k_BT)-1) \tag{8}$$

(according to the experiment there is only one magnon branch up to the Neel temperature), then differentiating F with respect to $\langle n_k\rangle$ and equating the derivative to zero we get the implicit equation for the temperature dependent magnon energy

$$\varepsilon_k(T) = \varepsilon^{(0)}_k\{1+c_k/2S-[(A_k-|\gamma_k|^2)/E^2_kSN_0]\sum_q(A_q-|\gamma_q|^2)\,\langle n_q\rangle/E_q+$$
$$+[|\gamma_k|^2/E^2_kSN_0]\sum_q|\gamma_q|^2\langle n_q\rangle/E_q-\mathrm{Re}\,[(\gamma_k/E^2_kSN_0)\sum_q\gamma^*_q\gamma_{q-k}\langle n_q\rangle/E_q]+$$
$$+(\tilde{\eta}/\eta)\,[A_k(\zeta_k-1)/E^2_kSN_0]\sum_q A_q(\zeta_q-1)\,\langle n_q\rangle/E_q\}. \tag{9}$$

The summation $(1/N_0)\sum_q$ can be changed to the intergration over the Brillouin zone. Because the functions under the summation sign have the property that $f(q+\mathscr{K}) = f(q)$ where $\mathscr{K}$ is any reciprocal lattice vector, we can instead integrate over the unit cell of the reciprocal lattice where each of the q_1, q_2, q_3 ($\boldsymbol{q} = q_1\boldsymbol{b}_1+q_2\boldsymbol{b}_2+q_3\boldsymbol{b}_3$) changes from 0 to 1 ($\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ are the primitive vectors of the reciprocal lattice)

$$(1/N_0)\sum_q(\ldots)\to\int_0^1\int_0^1\int_0^1(\ldots)dq_1dq_2dq_3. \tag{10}$$

The term in (9) which is proportional to $(\tilde{\eta}/\eta)\cong -0.005$ for the case of Cr_2O_3 will be omitted in the following part of the paper.

From our formulae we can get as a special case the result of Bloch [3] for a simple two-sublattice antiferromagnet with one interaction constant.

$$\tilde{\varepsilon}_k(T) = \tilde{\varepsilon}_k^{(0)}[1+\tilde{c}/2S-(1/SN_0)\sum_q (1-\tilde{\gamma}_q^2)^{1/2}\langle n_q\rangle];$$

$$\tilde{\varepsilon}^{(0)} = 2S|J|z\tilde{E}_k; \quad \tilde{E}_k = (1-\tilde{\gamma}_k^2)^{1/2};$$

$$\tilde{c} = (1/N_0)\sum_q (1-\tilde{E}_q); \quad \tilde{\gamma}_k = (1/z)\sum_\delta \exp(i\boldsymbol{k}\cdot\boldsymbol{\delta})$$

z = the number of nearest neighbours, $\boldsymbol{\delta}$ are their position vectors.

This formula can be obtained from ours if we make the following replacement: $A_k \to 1$, $\gamma_k \to \tilde{\gamma}_k$, $(-2S\eta) \to 2S|J|z$ and make use of the fact that in such a simple case

$$(\tilde{\gamma}_k/E_k^2)\sum_q (\tilde{\gamma}_q/\tilde{E}_q)\tilde{\gamma}_{q-k} = (\tilde{\gamma}_k^2/\tilde{E}_k^2)\sum_q (\tilde{\gamma}_q^2/\tilde{E}_q)$$

and similarly for the analogous summation including $\langle n_q\rangle$. In this simple case one can write

$$\tilde{\varepsilon}_k(T) = \tilde{\varepsilon}_k^{(0)}\alpha(T)$$

and $\alpha(T)$ does not dependend on k. This very much simplifies the calculation of $\tilde{\varepsilon}_k(T)$.

4. The method of Nagai applied to Cr_2O_3

The temperature-dependent magnon energies can also be obtained in the approximation first introduced by Nagai [4]. Below we shall apply this method in the case of Cr_2O_3. The procedure is as follows. We start with the Hamiltonian obtained in the first part of this paper after the second transformation (4)–(4c). For simplification we shall omit in (4c) terms including $\tilde{\eta}$ (see the remark beneath formula (10)). Now the biquadratic terms in the Hamiltonian (4) are replaced by the bilinear ones in such a way that the whole Hamiltonian (4) is approximated by the expression:

$$\mathscr{H} = \text{const.} + \sum_k \mathscr{A}'_k(a_k^\dagger a_k + b_k^\dagger b_k) + \mathscr{B}'_k a_k b_k + \mathscr{B}'^*_k a_k^\dagger b_k^\dagger. \tag{11}$$

This is achieved by replacement of the pairs of operators in (4c) through their expectation values calculated in the eigenstates of the total approximate Hamiltonian (11).

The calculation of the averages is performed using the formula

$$\langle a_k b_k\rangle = (\mathrm{Tr}\, a_k b_k \exp(-\mathscr{H}/k_B T))/\mathrm{Tr}\exp(-\mathscr{H}/k_B T) \tag{12}$$

where $\mathscr{H}$ is the total Hamiltonian (11) in the diagonalized form:

$$\mathscr{H} = \text{const.} + \sum_k \varepsilon_k(T)\,(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k) \tag{13}$$

so that

$$\langle \alpha_k^\dagger\alpha_k\rangle = \langle \beta_k^\dagger\beta_k\rangle = 1/(\exp(\varepsilon_k(T)/k_B T)-1) = \langle n_k\rangle. \tag{14}$$

In order to apply (14) in the calculations of the averages we must introduce a diagonalization procedure transforming (11) to (13). We can write this transformation immediately if we assume for a moment that we know $\mathscr{A}'_k$, $\mathscr{B}'_k$. Namely the formulae for transformation are analogous to those introduced already in (5). The difference is only in the coefficients of the transformation which we shall now call $L_k^{(1)}$, $L_k^{(2)}$ instead of the previous $l_k^{(1)}$, $l_k^{(2)}$.

$$a_k^\dagger = L_k^{(1)}\alpha_k^\dagger + L_k^{(2)}b_k; \qquad b_k^\dagger = L_k^{(2)}\alpha_k + L_k^{(1)}\beta_k^\dagger$$

$$a_k = L_k^{(1)*}\alpha_k + L_k^{(2)*}b_k^\dagger; \qquad b_k = L_k^{(2)*}\alpha_k^\dagger + L_k^{(1)*}\beta_k \tag{15}$$

$$L_k^{(1),(2)} = \pm[(\mathscr{A}'_k \pm \varepsilon_k(T))/2\varepsilon_k(T)]^{1/2} \exp(i\varnothing_k/2)$$

$$\exp(i\varphi_k) = \mathscr{B}'_k/|\mathscr{B}'_k|; \qquad |L_k^{(1)}|^2 - |L_k^{(2)}|^2 = 1$$

$$\varepsilon_k(T) = [\mathscr{A}'^2_k - |\mathscr{B}'_k|^2]^{1/2} \overset{\mathrm{df}}{=} (-2S\eta)E_k(T). \tag{16}$$

Using these formulae we can calculate the averages necessary to obtain the expressions for $\mathscr{A}'_k$ and $\mathscr{B}'_k$.

$$\langle a_k b_k\rangle = \langle (L_k^{(1)*}\alpha_k + L_k^{(2)*}\beta_k^\dagger)(L_k^{(2)*}\alpha_k^\dagger + L_k^{(1)*}\beta_k)\rangle =$$

$$= -\mathscr{B}'^*_k(\langle n_k\rangle + 1/2)(\varepsilon_k(T) \tag{17}$$

$$\langle a_k^\dagger b_k^\dagger\rangle = -\mathscr{B}'_k(\langle n_k\rangle + 1/2)/\varepsilon_k(T) \tag{18}$$

$$\langle a_k^\dagger a_k\rangle = \langle b_k^\dagger b_k\rangle = \mathscr{A}'_k(\langle n_k\rangle + 1/2)/\varepsilon_k(T) - 1/2. \tag{19}$$

The rest of the averages equals zero because they do not contain operators of the form $\alpha_k^\dagger\alpha_k$ or $\beta_k^\dagger\beta_k$.

Now we turn again to the beginning of our procedure, namely to the formula (11) and write this formula explicitly. Instead of $\mathscr{H}_{\mathrm{II}}^{(2)}$ (4c) we write approximately

$$\mathscr{H}_{\mathrm{II}}^{(2)} \cong (2\eta/N_0)\,[\sum_{kq} \langle b_q^\dagger b_q\rangle a_k^\dagger a_k + \langle a_q^\dagger a_q\rangle b_k^\dagger b_k +$$

$$+ \sum_{kq} \langle a_q^\dagger b_q^\dagger\rangle \gamma_{k-q} a_k b_k + \langle a_q b_q\rangle \gamma_{q-k} a_k^\dagger b_k^\dagger] +$$

$$+ (\eta/N_0)\,[\sum_{kq} \langle a_q b_q\rangle \gamma_q a_k^\dagger a_k + \langle a_q b_q\rangle \gamma_q b_k^\dagger b_k +$$

$$+ \sum_{kq} \langle a_q^\dagger a_q\rangle \gamma_k a_k b_k + \langle b_q^\dagger b_q\rangle \gamma_k a_k b_k + \text{h.c.}\,]. \tag{20}$$

Formula (20) is obtained from (4c) replacing each pair of operators through an average. Only those terms from (4c) are taken into account for which at least one pair of operators gives an average different from zero. Combining formulae (4b), (11), and (20) we get

$$\mathscr{A}'_k = \mathscr{A}_k + \eta\{(2/N_0)\sum_q \langle a_q^\dagger a_q\rangle + (1/N_0)\sum_q \langle a_q b_q\rangle \gamma_q + \langle a_q^\dagger b_q^\dagger\rangle \gamma_q^*\} \tag{21a}$$

$$\mathscr{B}'_k = \mathscr{B}_k + \eta\{(2/N_0)\sum_q \langle a_q^\dagger b_q^\dagger\rangle \gamma_{k-q} + (2/N_0)\gamma_k \sum_q \langle a_q^\dagger a_q\rangle\}. \tag{21b}$$

Now we can formulate the final result. The temperature dependent magnon energies are obtained using formula (16). This contains the averages which must be calculated from the selfconsistent equations (17)–(19). These equations can be very much simplified if we introduce the following definitions.

First, in complete analogy to the Nagai paper [4] we introduce the parameter u:

$$u \stackrel{\mathrm{df}}{=} (1/SN_0) \sum_q \langle a_q^\dagger a_q \rangle . \tag{22}$$

Besides this, Nagai defined in his paper one other parameter, w. In our case we have to introduce instead four parameters w_1, w_2, w_3, w_5 connected as we shall see with interaction constants J_1, J_2, J_3. J_5 (J_4 does not play here the same role as the other interaction constants because we have excluded some terms proportional to $\tilde{\eta} = 6J_4$). The appearence of one perameter "w" in Nagai paper is connected with one interaction constant which he took into account.

We assume the following definitions of the parameters:

$$w_1 \stackrel{\mathrm{df}}{=} (1/SN_0) \sum_q \langle a_q^\dagger b_q^\dagger \rangle \exp(-i\boldsymbol{q}\cdot\boldsymbol{v})$$

$$w_2 \stackrel{\mathrm{df}}{=} (1/SN_0) \sum_q \langle a_q^\dagger b_q^\dagger \rangle \exp(-i\boldsymbol{q}\cdot\boldsymbol{v}+i\boldsymbol{q}\cdot\boldsymbol{a}_1)$$

$$w_3 \stackrel{\mathrm{df}}{=} (1/SN_0) \sum_q \langle a_q^\dagger b_q^\dagger \rangle \exp(-i\boldsymbol{q}\cdot\boldsymbol{v}+i\boldsymbol{q}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_2))$$

$$w_5 \stackrel{\mathrm{df}}{=} (1/SN_0) \sum_q \langle a_q^\dagger b_q^\dagger \rangle \exp(-i\boldsymbol{q}\cdot\boldsymbol{v}+i\boldsymbol{q}(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3)) . \tag{23}$$

Now we can write $\mathscr{B}_k'$ in the following form (the details are given elsewhere [8])

$$\begin{aligned}\mathscr{B}_k' = (-2S\eta)\gamma_k(\alpha_1\alpha_2\alpha_3\alpha_5) = (-2S\eta)\exp(i\boldsymbol{k}\cdot\boldsymbol{v})\{\alpha_1+ \\ +\alpha_2[\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_1)+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_2)+\exp(-i\boldsymbol{k}\cdot\boldsymbol{a}_3)]+ \\ +\alpha_3[\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_2))+\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_1+\boldsymbol{a}_3))+\exp(-i\boldsymbol{k}\cdot(\boldsymbol{a}_2+\boldsymbol{a}_3))]+ \\ +\alpha_5[\exp(-i\boldsymbol{k}(\boldsymbol{a}_1+\boldsymbol{a}_2+\boldsymbol{a}_3))]\}\end{aligned} \tag{24}$$

(compare with (4d)), where we have introduced the following parameters:

$$\alpha_1 \stackrel{\mathrm{df}}{=} j_1(1-u-w_1), \quad \alpha_2 \stackrel{\mathrm{df}}{=} j_2(1-u-w_2), \quad \alpha_3 \stackrel{\mathrm{df}}{=} j_3(1-u-w_3),$$

$$\alpha_5 \stackrel{\mathrm{df}}{=} j_5(1-u-w_5). \tag{25}$$

Similarly to $\mathscr{B}_k'$ we can express $\mathscr{A}_k'$:

$$\mathscr{A}_k' = (-2S\eta)A_k'$$

$$A_k' = \alpha_1+3\alpha_2+3\alpha_3+\alpha_5+\alpha-6j_4(1-\zeta_k). \tag{26}$$

Now, using formula (16) and the parameters α_1, α_2, α_3, α_5 we can write the temperature dependent magnon energy

$$\varepsilon_k(T) = (-2S\eta)E_k(T) =$$

$$= (-2S\eta)\ \{[\alpha_1+3\alpha_2+3\alpha_3+\alpha_5+\alpha-6j_4(1-\zeta_k)]^2-|\gamma_k(\alpha_1\alpha_2\alpha_3\alpha_5)|^2\}^{1/2} \tag{27}$$

$$|\gamma_k(\alpha_1\alpha_2\alpha_3\alpha_5)|^2 = \alpha_1^2+2\alpha_2^2+3\alpha_3^2+\alpha_5^2+$$

$$+(2\alpha_1\alpha_2+4\alpha_2\alpha_3+2\alpha_3\alpha_5)\,(\cos 2\pi q_1+\cos 2\pi q_2+\cos 2\pi q_3)+$$

$$+(2\alpha_1\alpha_3+2\alpha_2\alpha_5)\,(\cos 2\pi(q_1+q_2)+\cos 2\pi(q_1+q_3)+\cos 2\pi(q_2+q_3))+$$

$$+(2\alpha_2^2+2\alpha_3^2)\,(\cos 2\pi(q_1-q_2)+\cos 2\pi(q_1-q_3)+\cos 2\pi(q_2-q_3))+$$

$$+2\alpha_2\alpha_3(\cos 2\pi(q_1-q_2-q_3)+\cos 2\pi(q_2-q_1-q_3)+\cos 2\pi(q_3-q_1-q_2))+$$

$$+2\alpha_1\alpha_5\cos 2\pi(q_1+q_2+q_3).$$

From (23) we get the following self-consistent equations for the new parameters (replacing summations through integrations):

$$\alpha_1 = j_1\{1+1/2S-(1/S)\int_0^1\int_0^1\int_0^1 [\alpha+(3\alpha_2-6j_4)\,(1-\cos 2\pi q_1)+$$

$$+3\alpha_3(1-\cos 2\pi(q_1+q_2))+\alpha_5(1-\cos 2\pi(q_1+q_2+q_3))]\times$$

$$\times(\langle n_q\rangle+1/2)/E_q(T)dq_1dq_2dq_3\}. \tag{28}$$

$$\alpha_2 = j_2\{1+1/2S-(1/S)\int_0^1\int_0^1\int_0^1 [\alpha+(\alpha_1-6j_4)\,(1-\cos 2\pi q_1)+$$

$$+2\alpha_2(1-\cos 2\pi(q_1-q_2))+\alpha_3(3-2\cos 2\pi q_1-\cos 2\pi(q_1+q_2-q_3))+$$

$$+\alpha_5(1-\cos 2\pi(q_1+q_2))]\times$$

$$\times(\langle n_q\rangle+1/2)/E_q(T)dq_1dq_2dq_3\}. \tag{29}$$

$$\alpha_3 = j_3\{1+1/2S-(1/S)\int_0^1\int_0^1\int_0^1 [\alpha+(\alpha_5-6j_4)\,(1-\cos 2\pi q_1)+$$

$$+2\alpha_3(1-\cos 2\pi(q_1-q_2))+\alpha_2(3-2\cos 2\pi q_1-\cos 2\pi(q_1+q_2-q_3))+$$

$$+\alpha_1(1-\cos 2\pi(q_1+q_2))]\times$$

$$\times(\langle n_q\rangle+1/2)/E_q(T)dq_1dq_2dq_3\}. \tag{30}$$

$$\alpha_5 = j_5\{1+1/2S-(1/S)\int_0^1\int_0^1\int_0^1[\alpha+(3\alpha_3-6j_4)(1-\cos 2\pi q_1)+$$
$$+3\alpha_2(1-\cos 2\pi(q_1+q_2))+\alpha_1(1-\cos 2\pi(q_1+q_2+q_3))]\times$$
$$\times(\langle n_q\rangle+1/2)/E_q(T)dq_1dq_2dq_3\}. \tag{31}$$

$$\langle n_q\rangle = 1/[\exp(-2S\eta E_q(T)/k_BT)-1] = 1/[\exp(E_q(t)/t)-1],$$
$$t \overset{\text{df}}{=} k_BT/(-2S\eta). \tag{32}$$

Comparing this result with the formula (5a), we see that the only difference is in replacing J_i through $J_i(1-u-w_i)$, $i = 1, 2, 3, 5$ which recalls the Keffer and Loudon result [9, 10] (renormalization of the interaction constants).

There is a connection between the result for $\varepsilon_k(T)$ obtained by the method of Bloch and that obtained by the method of Nagai. One can see it expanding (27), treating u, w_1, w_2, w_3, w_5 as small parameters:

$$\varepsilon_k(T) \cong [\varepsilon_k(T)]_{u=\ldots=w_5=0}+[\partial\varepsilon_k(T)/\partial u]_{u=\ldots=w_5}u+\ldots+[\partial\varepsilon_k(T)/\partial w_5]_{u=\ldots=w_5=0}w_5.$$

Now, putting in the place of u, w_1, w_2, w_3, w_5 their values from the selfconsistent equations (23), assuming on the righthand side of those equations $u = w_1 = w_2 = w_3 = w_5 = 0$, but keeping $\varepsilon_k(T)$ in the formula for $\langle n_k\rangle$, one obtaines our previous formula for temperature dependent magnon energy (9).

5. *Numerical results*

We have obtained numerical results for $\varepsilon_k(T)$ using both methods [3, 4] (in the following part of the paper we shall use the notation $\varepsilon_k^B(T)$ for $\varepsilon_k(T)$ as given by the formula (9), $\varepsilon_k^N(T)$ for $\varepsilon_k(T)$ as given by the formula (27)), and compared the results with the experimental data of Samuelsen [5, 6]. He has measured in detail the magnon dispersion relations for Cr_2O_3 at 78 K [6] and made a fit of the experimental curves to the theoretical formula for the energy, calculated in the noninteracting spin wave approximation which was the same as our formula (5a) (in the case when the fit was done using five interaction constants). Samuelsen obtained in this way the values for J_1, J_2, J_3, J_4, J_5. The anisotropy constant G was taken from other experiments, and $\alpha = G/(-2S\eta) \cong 8\cdot10^{-5}$.

In order to obtain numerical results we started with (27). Using the similarity of the functional form of (27) and (5a) we could obtain comparatively easily new values for $J_1, \ldots J_5$ which gave good agreement between the experimental curves at 78 K and $\varepsilon_k^N(T)$ at the same temperature. Below, in Table II we give both sets of interaction constants,

TABLE II

Interaction constants for Cr_2O_3 (in meV)	J_1	J_2	J_3	J_4	J_5
Result of Samuelsen	−7.53	−3.41	−0.078	+0.017	−0.190
Result from the method of Nagai	−6.79	−3.33	−0.084	+0.017	−0.215

Samuelsen's and ours. The new interaction constants were used to obtain $\varepsilon_k^N(T)$ at higher temperatures and also in the formula for $\varepsilon_k^B(T)$.

In Fig. 2 we give three magnon dispersion curves as obtained by the Nagai method, *i.e.* $\varepsilon_k^N(T)$, in $\boldsymbol{b}_1$ (the same result would be in $\boldsymbol{b}_2$ or $\boldsymbol{b}_3$) direction ([110] in the notation of Samuelsen) for temperatures 78 K, 205 K, 291 K (T_N = 308 K), as well as the experimental

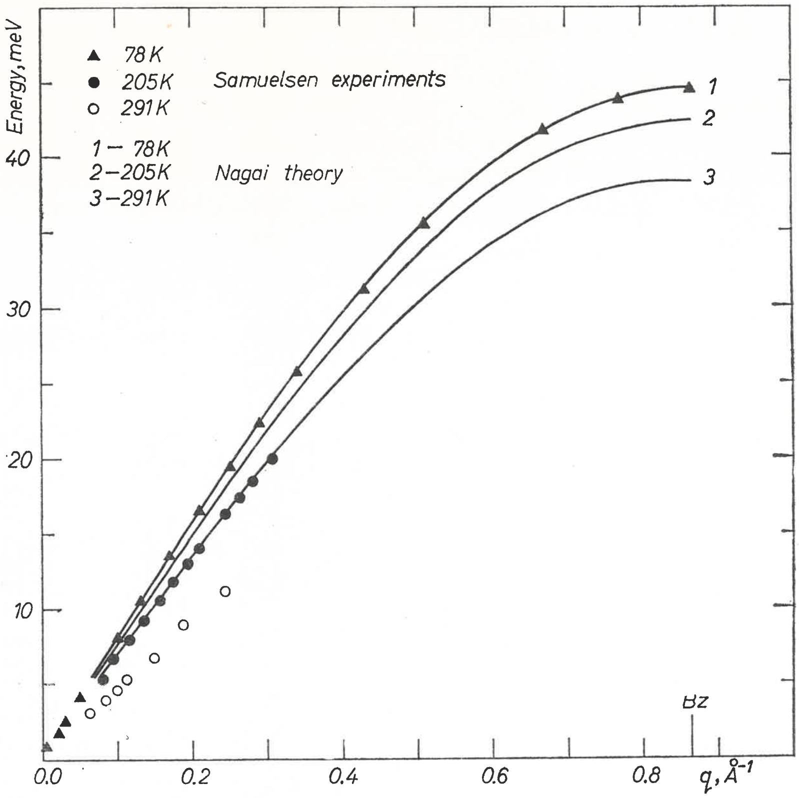

Fig. 2. The temperature dependent magnon energies for Cr_2O_3 as obtained by the method of Nagai, and the experimental results of Samuelsen [5, 6] at temperatures 78 K, 205 K, 291 K

results [5, 6]. The theoretical curves were obtained solving first selfconsistent equations (28)–(31) for the parameters $\alpha_1, \alpha_2, \alpha_3, \alpha_5$, and then using them in (27) to get $\varepsilon_k^N(T)$.

In Fig. 3 we show the temperature dependence of "the renormalizing factors of the interaction constants" $(1-u-w_i)$ $i = 1, 2, 3, 5$.

There exists the highest temperature, $t_{\max}^N$, at which the magnon energy becomes imaginary, so that we have no physical solution. We have estimated that this temperature is lying in the interval $0.60 < t_{\max}^N < 0.63$.

The computations were performed using Odra 1204 computer and the Simpson approximation procedure for integration, with the accuracy parameter for this procedure equal to 0.01.

The formula for temperature dependent magnon energies (9) as given by the method of Bloch can be written in an equivalent form which is more suitable for numerical calculations (see Appendix)

$$\varepsilon_k^B(T) = f_k^{(0)} + f_k^{(1)} D_1 + \ldots + f_k^{(5)} D_5 \tag{33}$$

where $f_k^{(i)}$ are functions of $\boldsymbol{k}$, not depending on $\varepsilon_k^B(T)$ and $D_j(j = 1, \ldots, 5)$ are integrals depending on $\varepsilon_k^B(T)$. Therefore we treat D_j as unknown, temperature- dependent parameters which we have to calculate selfconsistently. $D_j(T)$ calculated in this way should be put

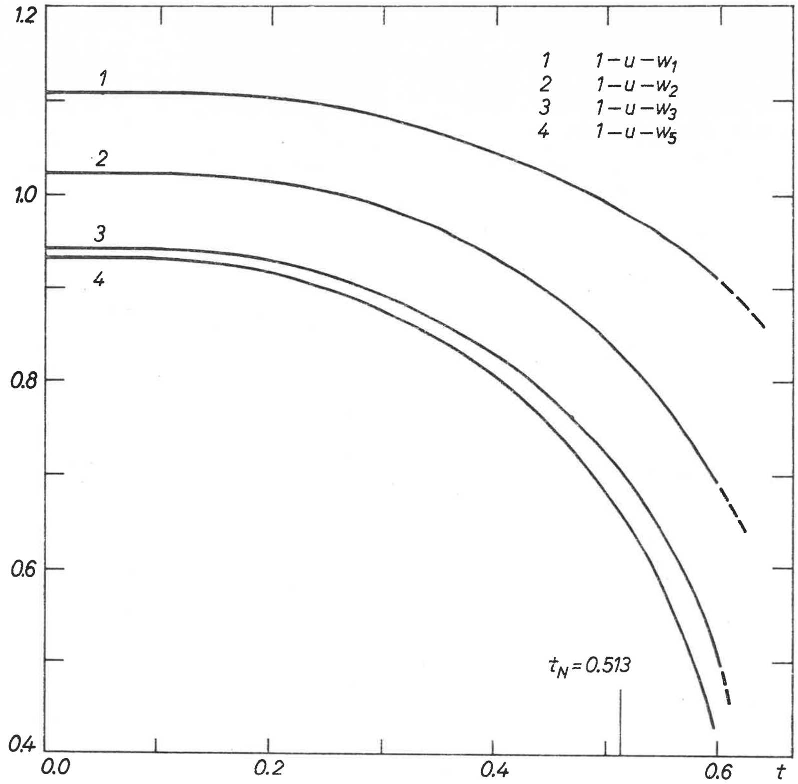

Fig. 3. The temperature dependence of the renormalizing factors of the interaction constants $(1-u-w_i)$ $i = 1, 2, 3, 5$, introduced and calculated for Cr_2O_3 according to the theory of Nagai

into formula (33) to obtain $\varepsilon_k^B(T)$. The energy curves $\varepsilon_k^B(T)$ calculated in this way for $\boldsymbol{k}$ in $\boldsymbol{b}_i$ $(i = 1, 2, 3)$ direction differ very little from $\varepsilon_k^N(T)$ for the whole considered temperature range. The approximate procedure we have used for integration allows us only to state that the values of $\varepsilon_k^B(T)$ are lying systematically lower than $\varepsilon_k^N(T)$, the difference being within few percent, so that we have not given the separate curves for $\varepsilon_k^B(T)$. Using Bloch method we have also found that there exists a temperature $t_{\max}^B$, above which there is no selfconsistent solution for the parameters D_j giving reasonable energy values. We have estimated that this temperature must lie approximately in the same temperature interval as $t_{\max}^N$.

6. *Discussion*

For some materials a good fit was obtained between the theory of Bloch or Nagai and experiments on magnetization, susceptibility and magnon dispersion curves for temperatures sometimes very near to the Neel or Curie temperature [11, 12, 13]. But in all these cases the value of T_N or T_C was low, not exceeding 100 K. In the case of $Cr_2O_3(T_N = 308\,K)$ we see that there is no agreement for temperatures as high as 205 K, 291 K. May be that for this case one should take into account the higher order terms of the Oguchi expansion, and may be also magnon-phonon interaction.

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APPENDIX

We shall show here how to obtain formula (33) for $\varepsilon_k^B(T)$ starting from the previous formula (9).

In the formula (9) we must introduce γ_{k-q} according to the definition (4d) and take the terms depending on $\boldsymbol{k}$ outside the summation over $\boldsymbol{q}$. A straightforward but tedious calculations show that we can write (9) in the form:

$$\varepsilon_k^B(T) = \varepsilon_k^{(0)}\{1+(1/2SE_k^2)\,[(A_k-|\gamma_k|^2)-(A_k-|\gamma_k|^2)D_1+|\gamma_k|^2D_2-$$
$$-j_1F_k(j_1j_2j_3j_5)D_3-j_2G_k(j_1j_2j_3j_5)D_4-$$
$$-j_3G_k(j_5j_3j_2j_1)D_5-j_5F_k(j_5j_3j_2j_1)D_6]\}\,.$$

where

$$D_1 = (1/N_0)\sum_q (2\langle n_q\rangle+1)\,(A_q-|\gamma_q|^2)/E_q$$

$$D_2 = (1/N_0)\sum_q (2\langle n_q\rangle+1)\,|\gamma_q|^2/E_q$$

$$D_3 = (1/N_0)\sum_q F_q(j_1j_2j_3j_5)\,(2\langle n_q\rangle+1)/E_q$$

$$D_4 = (1/N_0)\sum_q G_q(j_1j_2j_3j_5)\,(2\langle n_q\rangle+1)/E_q$$

$$D_5 = (1/N_0)\sum_q G_q(j_5j_3j_2j_1)\,(2\langle n_q\rangle+1)/E_q$$

$$D_6 = (1/N_0)\sum_q F_q(j_5j_3j_2j_1)\,(2\langle n_q\rangle+1)/E_q$$

$$F_k(j_1j_2j_3j_5) = j_1+j_2(\cos 2\pi k_1+\cos 2\pi k_2+\cos 2\pi k_3)+$$
$$+j_3\,[\cos 2\pi(k_1-k_2)+\cos 2\pi(k_1-k_3)+\cos 2\pi(k_2-k_3)]+$$
$$+j_5\cos 2\pi(k_1+k_2+k_3),$$

$$G_k(j_1 j_2 j_3 j_5) = j_1(\cos 2\pi k_1 + \cos 2\pi k_2 + \cos 2\pi k_3) +$$
$$+ j_2 [3 + 2\cos 2\pi(k_1 - k_2) + 2\cos 2\pi(k_1 - k_3) + 2\cos 2\pi(k_2 - k_3)] +$$
$$+ j_3 [2\cos 2\pi k_1 + 2\cos 2\pi k_2 + 2\cos 2\pi k_3 + \cos 2\pi(k_1 - k_2 - k_3) + \cos 2\pi(k_2 - k_1 - k_3) +$$
$$+ \cos 2\pi(k_3 - k_1 - k_2)] + j_5 [\cos 2\pi(k_1 + k_2) + \cos 2\pi(k_1 + k_3) + \cos 2\pi(k_2 + k_3)],$$
$$(\boldsymbol{k} = k_1 \boldsymbol{b}_1 + k_2 \boldsymbol{b}_2 + k_3 \boldsymbol{b}_3).$$

Besides, there is a temperature independent relation between D_j's:

$$D_2 = j_1 D_3 + 3 j_2 D_4 + 3 j_3 D_5 + j_5 D_6$$

which follows from the fact that:

$$\{|\gamma_k|^2 (1/N_0) \sum_q (2\langle n_q \rangle + 1) |\gamma_q|^2 / E_q - \mathrm{Re}\, [\gamma_k (1/N_0) \sum_q (2\langle n_q \rangle + 1) \gamma_q^* \gamma_{q-k} / E_q]\}_{k=0} = 0$$

So, at the end, one can write $\varepsilon_k^B(T)$ in the form introduced in (33).

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