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QUANTUM MECHANICAL OPERATOR EQUIVALENTS AND MAGNETIC ANISOTROPY OF THE HEAVY RARE EARTH METALS

by

Oluf Danielsen

Danish Atomic Energy Commission
Research Establishment Risö
Physics Department

Abstract

A tensor operator formalism that in a convenient way describes the interactions of magnetic systems is treated. Further a creation operator and annihilation operator formalism describing the excited states of magnetic systems is introduced. On this background temperature laws of the magnetic anisotropy of the heavy rare earth metals are calculated. Further is the temperature dependence of the spin wave spectrum and thereby the temperature dependence of the spin wave energy gap of the heavy rare earth metals calculated.

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1. INTRODUCTION

In the theory of magnetism the operator equivalents method is well established. Stevens was the first to invent the operator equivalents method in crystal field calculations and he introduced a set of operators which have been widely used. These Stevens operators, denoted O_k^q, have the disadvantage of not having systematic transformation properties under rotations of the frame of coordinates. Another set of operators, the Racah operators, denoted $\tilde{O}_{k,q}$, are tensor operators and they therefore have systematic transformation properties. Both sets of operators are expressible as angular momentum operators. They are treated in chapter 2 together with relations connecting the two sets of operators.

In magnetic systems it is convenient to use the Holstein-Primakoff transformation to express the angular momentum operators in Bose operators. The angular momentum operators are tensor operators of rank one. The Holstein-Primakoff method is a cumbersome way to calculate tensor operators of rank higher than one in terms of Bose operators expressions. Therefore in chapter 3 we use another method to express the Racah operators in terms of Bose operators by formally expanding the Racah operators in a well ordered Bose operator series and match the matrix elements between corresponding states.

The magnetic properties of the heavy rare earths metals are described by the combination of indirect exchange interaction and crystals field effects. Because of their large orbital moments, the heavy rare earth-metals display large magnetostriction effects, that modify the magnetic anisotropy caused by the crystal field. In chapter 4 we perform a spin wave calculation of the temperature dependence of the single ion anisotropy and the single ion magnetostriction.

The anisotropy forces of the heavy rare earth metals cause the acoustic spin wave dispersion relation not to approach zero in the long wave length limit. This spin wave energy gap is temperature dependent. In chapter 5 the temperature dependence of the energy gap has been deduced from the temperature dependence of the spin wave spectrum and in chapter 6 the temperature dependence has been treated by means of a resonans theory.

On the basis of the microscopic calculations in chapter 4 of the temperature dependence of the single ion anisotropy and of the single ion magnetostriction the temperature dependence of the macroscopic anisotropy constants of the heavy rare earths has been calculated in chapter 7. By means of inelastic neutron scattering experiments performed at Risø a numerical calculation of the temperature dependence of the macroscopic anisotropy constants of terbium has been carried out in chapter 8.

2. QUANTUM MECHANICAL OPERATOR EQUIVALENTS

2.1. Introduction

The Operator Equivalents Method was developed by Stevens[1], when he determined the matrix elements of crystal field potentials for some rare earth ions. The eigenfunctions of a rare earth ion can conveniently be written as $|\, 4\, f^n;\ \underline{L}\ \underline{S}\ \underline{J}\ \underline{J}_z \rangle$, n being the number of 4f-electrons, $\underline{L}$ the total orbital angular momentum, $\underline{S}$ the total spin angular momentum, $\underline{J} = \underline{L} + \underline{S}$ the total angular momentum and J_z the z-component of $\underline{J}$. A direct calculation of the matrix elements of the crystalfield potential $W_c(x, y, z)$ requires a decomposition of the eigenfunctions in determinantal product states of 4f one electron states. This is a tedious procedure and instead of doing so the operator equivalents method is used. Given the crystal field potential in Cartesian coordinates the operator equivalent of $W_c(x, y, z)$ is found by replacing x, y, z by the respective Cartesian components of $\underline{J}$[x]: J_x, J_y, J_z taking into account the noncommutation of J_x, J_y and J_z. In this way an operator is formed with the same transformation properties under rotation as the potential. The method depends on the fact that within a manifold of states for which $\underline{J}$ is constant there are simple relations (multiplicative factors) between the matrix elements of the crystal field potential calculated directly and by use of the angular momentum operators. These multiplicative factors are determined by returning to the direct integration method using single electron wavefunctions by using fractional parentage coefficients. The Stevens method of obtaining the operator equivalents are thus difficult. A more direct determination of the operator equivalents can be given on the basis of the tensor operator formalism developed by Racah[2].

2.2. Racah Operator Equivalents, $\tilde{O}_{K,q}$

A set of irreducible tensor operators are defined through their transformation properties. The Racah operators are irreducible tensor operators, which means that the set of 2K + 1 operators $\tilde{O}_{K,q}$ (q = K, K-1, K-2, ..., -K) transform under rotations of the frame of coordinates (through the Euler angles α, β, γ) as $\sqrt{\frac{4\pi}{2K+1}}$ times the spherical harmonics, $Y_{K,q}(\theta, \varphi)$ namely

$$\mathcal{D}(\alpha,\beta,\gamma)\, \tilde{O}_{K,q}\, \mathcal{D}(\alpha,\beta,\gamma)^{-1} = \sum_{q'=-K}^{q'=K} \tilde{O}_{K,q'}\, \mathcal{D}^{(K)}_{q'q}(\alpha,\beta,\gamma) \tag{2.1}$$

x) J is here used to denote a generalized angular momentum

The matrix elements of the rotation operator $D(\alpha,\beta,\gamma)$ are

$$D^{(K)}_{q'q}(\alpha,\beta,\gamma) = \langle Kq' | D(\alpha,\beta,\gamma) | Kq \rangle = e^{-iq'\alpha}\, d^{(K)}_{q'q}(-\beta)\, e^{-iq\gamma} \tag{2.2}$$

where

$$d^{(K)}_{q'q}(\beta) = \sqrt{\frac{(K+q')!\,(K-q')!}{(K+q)!\,(K-q)!}} \times \sum_{\sigma} \binom{K+q}{K-q'-\sigma}\binom{K-q}{\sigma} (-1)^{K-q'-\sigma} \left(\cos\frac{\beta}{2}\right)^{2\sigma+q'+q} \left(\sin\frac{\beta}{2}\right)^{2K-q'-q-2\sigma} \tag{2.3}$$

(the summation is over all positive σ such that the factorial terms are non negative).

Since the operators of total angular momentum are multiples of the infinitesimal rotation operators, we may replace the unitary transformation on the left by a commutator, giving for any component of angular momentum J_α, Edmonds[3]

$$[J_\alpha, \tilde{O}_{K,q}] = \sum_{q'=-K}^{q'=K} \tilde{O}_{K,q'} \langle Kq' | J_\alpha | Kq \rangle \tag{2.4}$$

Using the commutation relations of the components of the angular momenta J_α we find the original definition of the irreducible tensor operators given by Racah[2]

$$[J^{\pm}, \tilde{O}_{K,q}] = \sqrt{K(K+1) - q(q\pm 1)}\ \tilde{O}_{K,q\pm 1} \tag{2.5}$$

$$[J_z, \tilde{O}_{K,q}] = q\ \tilde{O}_{K,q} \tag{2.6}$$

The Racah operators in terms of angular momentum operators J_x, J_y, J_z can be obtained from the $[J^-, \tilde{O}_{K,q}]$ commutator relation if the operator with maximum q value, namely $q = K$, is known. The $\tilde{O}_{KK}$ operator is calculated using the Stevens equivalents method on the spherical harmonic $Y_{KK}(\theta,\varphi)$ expressed in Cartesian coordinates.

For the spherical harmonic $Y_{KK}(\theta,\varphi)$ we find, Edmonds[3])

$$Y_{KK}(\theta,\varphi) = (-1)^K \sqrt{\frac{2K+1}{4\pi(2K)!}}\; P_K^K(\cos\theta)\, e^{iK\varphi} \tag{2.7}$$

According to Jahnke and Emde[4]) the associated Legendre functions $P_K^q(\cos\theta)$ give for $q = K$

$$P_K^K(\cos\theta) = \frac{(2K)!}{2^K K!}\,(\sin\theta)^K \tag{2.8}$$

Introducing Cartesian coordinates we find from the two relations (2.7) and (2.8)

$$Y_{KK}(\theta,\varphi) = \frac{(-1)^K}{2^K (K)!}\sqrt{\frac{(2K+1)!}{4\pi}}\,(\sin\theta)^K e^{iK\varphi}$$

$$= \frac{(-1)^K}{2^K K!}\sqrt{\frac{(2K+1)!}{4\pi}}\;\left(\frac{x+iy}{r}\right)^K$$

Multiplying by $\sqrt{\frac{4\pi}{2K+1}}$ and replacing $\frac{x+iy}{r}$ by $J_x + i\,J_y = J^+$ we find $\tilde{O}_{KK}$

$$\tilde{O}_{K,K} = \frac{(-1)^K}{2^K K!}\sqrt{(2K)!}\;(J^+)^K \tag{2.9}$$

The operators $\tilde{O}_{K,-q}$ are obtained by means of the relation

$$\tilde{O}_{K,-q} = (-1)^q\,\tilde{O}_{K,q}^{\dagger} \tag{2.10}$$

The Racah operators have earlier been tabulated for all values of K up to K = 6 by Buckmaster[5]) and Smith and Thornley[6]), and up to K = 7 by Buckmaster et al[7]). In table (1) the Racah operators for all values of K up to K = 8 are tabulated based on calculations done by Danielsen and Lindgård[8]).

The matrix element of a Racah operator is determined within a system described by a state vector which is a simultaneous eigenvector of the angular momentum operators $\underline{J}^2$ and J_z. In Dirac's braket notation the eigenvector is given by $| J\, m \rangle$. The matrix element within a manifold of given angular momentum J is, Racah[2] and Edmonds[3]

$$\langle J m | \tilde{O}_{K,q} | J m' \rangle = (-1)^{J-m} \begin{pmatrix} J & K & J \\ -m & q & m' \end{pmatrix} \langle J \| \tilde{O}_K \| J \rangle \tag{2.11}$$

The factorization of the matrix element of the Racah operator in a reduced matrix element $\langle J \| \tilde{O}_K \| J \rangle$ independent of m and a 3j-symbol containing the m-dependence or the rotational dependence of the matrix element is a consequence of the Wigner-Eckart Theorem. It should be noted that a tensor operator in general is characterized by its reduced matrix element, here $\langle J \| \tilde{O}_K \| J \rangle$ for the Racah operators. In appendix 1 it is shown that the reduced matrix element is

$$\langle J \| \hat{O}_K \| J \rangle = \frac{1}{2^K} \sqrt{\frac{(2J+K+1)!}{(2J-K)!}} \tag{2.12}$$

Numerical values of the matrix elements have been calculated by Hutchings[9] and by Birgeneau[10]. Two Racah operators either commute or they do not commute. If the operators are acting on different parts of the system, say spin and orbit, they commute. If they act on the same dynamical variable, the commutator relation is not in general zero. For two non-commuting Racah operators the commutator relation has been calculated in appendix 2.

$$[\tilde{O}_{K_1,q_1}(i), \tilde{O}_{K_2,q_2}(i)] = \sum_{q_3=-K_3}^{K_3} \sum_{K_3=|K_1-K_2|}^{K_1+K_2} \left((-1)^{K_1+K_2+K_3} - 1\right)(2K_3+1) \begin{pmatrix} K_1 & K_2 & K_3 \\ q_1 & q_2 & q_3 \end{pmatrix} \times$$

$$\times \begin{Bmatrix} K_1 & K_2 & K_3 \\ J & J & J \end{Bmatrix} \frac{\langle J \| \tilde{O}_{K_1}(i) \| J \rangle \langle J \| \tilde{O}_{K_2}(i) \| J \rangle}{\langle J \| \tilde{O}_{K_3}(i) \| J \rangle} \tilde{O}^{\dagger}_{K_3,q_3}(i) \tag{2.13}$$

here { } denote a 6j-symbol.
For two commuting Racah operators we immediately have

$$[\tilde{O}_{K_1,q_1}(i), \tilde{O}_{K_2,q_2}(j)] = 0 \tag{2.14}$$

A proper tensor algebra of the Racah operators also include tensor products, scalar products and matrix elements of tensor products. The tensor product of two non-commuting Racah operators is defined by, Racah[2] and Judd[11]

$$\left(\tilde{O}^{(K_1)}\tilde{O}^{(K_2)}\right)^{(K)}_{Q} = \sum_{q_1=-K_1}^{K_1}\sum_{q_2=-K_2}^{K_2}(-1)^{K_2-K_1-Q}\sqrt{2K+1}\begin{pmatrix} K_1 & K_2 & K \\ q_1 & q_2 & -Q \end{pmatrix}\tilde{O}_{K_1 q_1}(i)\tilde{O}_{K_2 q_2}(i) \tag{2.15}$$

and for the scalar product of two non-commuting Racah operators we have

$$\left(\tilde{O}^{(K)}_{i}\tilde{O}^{(K)}_{i}\right) = (-1)^{K}\sqrt{2K+1}\;\left(\tilde{O}^{(K)}\tilde{O}^{(K)}\right)^{(0)}_{0} \tag{2.16}$$

which means that the scalar product is proportional to the zero-order tensor product. The matrix element of the tensor product of two non-commuting Racah operators is

$$\langle Jm|\left(\tilde{O}^{(K_1)}\tilde{O}^{(K_2)}\right)^{(K)}_{Q}|Jm'\rangle = (-1)^{J-m}\begin{pmatrix} J & K & J \\ -m & Q & m' \end{pmatrix}\langle J\|\left(\tilde{O}^{(K_1)}\tilde{O}^{(K_2)}\right)^{(K)}_{Q}\|J\rangle \tag{2.17}$$

The entering reduced matrix element is

$$\langle J\|\left(\tilde{O}^{(K_1)}\tilde{O}^{(K_2)}\right)^{(K)}_{Q}\|J\rangle = (-1)^{K}\sqrt{2K+1}\begin{Bmatrix} K_1 & K_2 & K \\ J & J & J \end{Bmatrix}\langle J\|\tilde{O}_{K_1}(i)\|J\rangle\langle J\|\tilde{O}_{K_2}(i)\|J\rangle \tag{2.18}$$

The tensor product of two commuting Racah operators is defined by

$$\left\{\tilde{O}^{(K_1)}\tilde{O}^{(K_2)}\right\}^{(K)}_{Q} = \sum_{q_1=-K_1}^{K_1}\sum_{q_2=-K_2}^{K_2}(-1)^{K_2-K_1-Q}\sqrt{2K+1}\begin{pmatrix} K_1 & K_2 & K \\ q_1 & q_2 & -Q \end{pmatrix}\tilde{O}_{K_1 q_1}(i)\,\tilde{O}_{K_2 q_2}(j) \tag{2.19}$$

and the scalar product of two commuting Racah operators turns out to be

$$\left(\tilde{O}^{(K)}_{i}\tilde{O}^{(K)}_{j}\right) = (-1)^{K}\sqrt{2K+1}\;\left\{\tilde{O}^{(K)}\tilde{O}^{(K)}\right\}^{(0)}_{0} \tag{2.20}$$

The matrix element of the tensor product of two commuting Racah operators is

$$\langle j_1 j_2 J m | \{\tilde{O}^{(K_1)} \tilde{O}^{(K_2)}\}^{(K)}_Q | j_1' j_2' J' m' \rangle = \tag{2.21}$$

$$(-1)^{J-m} \begin{pmatrix} J & K & J' \\ -m & Q & m' \end{pmatrix} \langle j_1 j_2 J \| \{\tilde{O}^{(K_1)} \tilde{O}^{(K_2)}\}^{(K)}_Q \| j_1' j_2' J' \rangle$$

with the reduced matrix element expressed through a 9j-symbol:

$$\langle j_1 j_2 J \| \{\tilde{O}^{(K_1)} \tilde{O}^{(K_2)}\}^{(K)}_Q \| j_1' j_2' J' \rangle =$$

$$\sqrt{(2J+1)(2J'+1)(2K+1)} \begin{Bmatrix} j_1 & j_2 & J \\ j_1' & j_2' & J' \\ K_1 & K_2 & K \end{Bmatrix} \langle j_1 \| \tilde{O}_{K_1}(i) \| j_1' \rangle \langle j_2 \| \tilde{O}_{K_2}(j) \| j_2' \rangle \tag{2.22}$$

All 3j- and 6j-symbols are calculated numerically by Rothenberg et al [12]

2.3. Stevens Operator Equivalents, O_K^q

The operator equivalents mentioned in the introduction defined by Stevens are related to the Racah tensor operators in essentially the same way as the tesseral harmonics are related to the spherical harmonics. The Racah operators namely transform under rotations of the frame of coordinates as the spherical harmonics, whereas the Stevens operators transform as do the tesseral harmonics. The Stevens operators O_K^q are expressed by the Racah operators, Danielsen and Lindgård[8]

$$O_K^q(c) = \frac{1}{\mathcal{K}_K^q} \sqrt{\frac{2K+1}{4\pi}} \frac{1}{\sqrt{2}} \left(\tilde{O}_{K,-q} + (-1)^q \tilde{O}_{K,q} \right) \tag{2.23}$$

$$O_K^q(s) = \frac{1}{\mathcal{K}_K^q} \sqrt{\frac{2K+1}{4\pi}} \frac{i}{\sqrt{2}} \left(\tilde{O}_{K,-q} - (-1)^q \tilde{O}_{K,q} \right) \tag{2.24}$$

$$O_K^0(c) = \frac{1}{\mathcal{K}_K^0} \sqrt{\frac{2K+1}{4\pi}} \, \tilde{O}_{K,0} \; ; \quad O_K^0(s) \equiv 0 \tag{2.25}$$

$\mathcal{K}_K^q$ are the normalization coefficients of the tesseral harmonics. The Stevens operators expressed as angular momentum operators are given in table (2) for all even values of K up to 8, and the $\mathcal{K}_K^q$-coefficients are given for K up to 8 in table (3).

3. RACAH OPERATOR EQUIVALENTS EXPANDED IN BOSE OPERATORS

3.1. Introduction

Until now the Racah operator equivalents have been expressed as angular momentum operators, table (1). When the operators are used for statistical mechanical calculations in quantum mechanical angular momentum systems such calculations are made difficult by the fact that the commutators between angular momenta are still operators, namely

$$[J_z, J^+] = J^+ \qquad (3.1)$$

$$[J_z, J^-] = -J^- \qquad (3.2)$$

$$[J^+, J^-] = 2J_z \qquad (3.3)$$

(in units of $\hbar$)

The fact that the z-component of the angular momentum J_z can only take $2J+1$ values and because of the kinematical length condition $\underline{J} \cdot \underline{J} = J(J+1)$ and the minimum equations $(J^+)^{2J+1} = 0$ and $(J^-)^{2J+1} = 0$ together with the form of the commutation relation statistics of spin systems and thereby a systematical perturbation theory are difficult to establish, Fogedby[13]. To avoid these difficulties the angular momentum operators are transformed into creation - and annihilation operators, (second quantization) either Bose operators or Fermi operators that have well-established statistics. In contrast with the angular momentum operators the Bose and Fermi operators obey commutation relations that result in c-numbers, namely for

Bose operators:

$$[a_j, a_l^+] = \delta_{jl} \; ; \; [a_j, a_l] = [a_j^+, a_l^+] = 0 \qquad (3.4)$$

and for

Fermi operators:

$$\{c_j, c_l^+\} = \delta_{jl}$$
$$\{c_j, c_l\} = \{c_j^+, c_l^+\} = 0 \qquad (3.5)$$

(where [,] denotes commutator and { , } denotes anticommutator).

3.2. Angular Momentum to Bose Operator Transformations

In magnetic systems where the Hamiltonian is expressible in angular momentum operators the eigen states are in semi-classical terms described as spin waves whereas in a quantum language the eigen states - the normal modes - are described as magnons. Various collective modes occurring in many-particle systems are Boson modes, and among these are the magnons, obeying Boson commutation relations and Bose statistics.

The idea of transforming an angular momentum operator into Bose operators was first carried out by Holstein and Primakoff[14]. Another transformation is the Dyson - Maleev transformation which in contradistinction to the Holstein - Primakoff transformation is non-hermitian. In the following we are going to consider such angular momentum to Bose operator transformations. The original Holstein - Primakoff transformation is

$$J_l^z = J - a_l^+ a_l = J - \hat{n}_l \qquad (3.6)$$

$$J_l^+ = \sqrt{2J}\sqrt{1 - \frac{a_l^+ a_l}{2J}}\, a_l = \sqrt{2J}\sqrt{1 - \frac{\hat{n}_l}{2J}}\, a_l \qquad (3.7)$$

$$J_l^- = \sqrt{2J}\, a_l^+ \sqrt{1 - \frac{a_l^+ a_l}{2J}} = \sqrt{2J}\, a_l^+ \sqrt{1 - \frac{\hat{n}_l}{2J}} \qquad (3.8)$$

The operator $\hat{n}_l$ is called the number operator and its eigenvalues n_l are the spin deviations of the l^{th} atom in the many particle system , n_l represents the difference between the z-component of the angular momentum of the l^{th} atom and its maximum value. Thinking of the square roots of the transformation as given by their Taylor expansions we have

$$a_l\sqrt{1-\frac{a_l^+a_l}{2J}} = \sqrt{1-\frac{a_l^+a_l+1}{2J}}\,a_l \tag{3.9}$$

$$a_l^+\sqrt{1-\frac{a_l^+a_l}{2J}} = \sqrt{1-\frac{a_l^+a_l-1}{2J}}\,a_l^+ \tag{3.10}$$

for which reason the commutation relation between J_l^+ and J_l^- turns out to be

$$\begin{aligned}
[J_l^+, J_l^-] &= J_l^+J_l^- - J_l^-J_l^+ \\
&= 2J\left\{\sqrt{1-\frac{a_l^+a_l}{2J}}\,a_la_l^+\sqrt{1-\frac{a_l^+a_l}{2J}} - a_l^+\left(1-\frac{a_l^+a_l}{2J}\right)a_l\right\} \\
&= 2J\left\{1-\frac{a_l^+a_l}{2J} + a_l^+\left(\sqrt{1-\frac{a_l^+a_l+1}{2J}}\right)^2 a_l - a_l^+a_l + \frac{a_l^+a_l^+a_la_l}{2J}\right\} \\
&= 2(J-a_l^+a_l) \\
&= 2J_l^z
\end{aligned} \tag{3.11}$$

which agrees with the angular momentum relation (3.3). The Holstein - Primakoff transformation is defined in the space of eigen-functions of the occupation numbers $n_l = 0, 1, 2, \ldots\ldots$ The subspace of functions of the occupation numbers $n_l \geq 2J + 1$ is called the non-physical space. The physical states are those for $n_l = 0, 1, 2, 3, \ldots\ldots, 2J$.

The 2J + 1 physical states may either be expressed as angular momentum states or as deviation states. Starting with the ground state the angular momentum states $|J, m\rangle$ are

$$|J,J\rangle,\ |J,J-1\rangle,\ |J,J-2\rangle, \cdots |J,J-n\rangle, \cdots |J,-J\rangle \tag{3.12}$$

while the deviation states $|n\rangle$ are

$$|0\rangle, |1\rangle, |2\rangle, \cdots |n\rangle, \cdots |2J+1\rangle \tag{3.13}$$

with the corresponding energy eigenvalues

$$E_0 < E_1 < E_2 < \cdots < E_n < \cdots < E_{2J+1} \tag{3.14}$$

The angular momentum operators act on the eigenstates, $|J, m\rangle$

$$J_z|J,m\rangle = m|J,m\rangle \quad ; m = J, J-1, J-2, \cdots, -J \tag{3.15}$$

$$J^+|J,m\rangle = \sqrt{(J-m)(J+m+1)}\ |J, m+1\rangle \tag{3.16}$$

$$J^-|J,m\rangle = \sqrt{(J+m)(J-m+1)}\ |J, m-1\rangle \tag{3.17}$$

while the creation and annihilation operators acting on their corresponding eigenstates give

$$a^+|n\rangle = \sqrt{n+1}\ |n+1\rangle \tag{3.18}$$

$$a|n\rangle = \sqrt{n}\ |n-1\rangle \tag{3.19}$$

Because of the closure of the Holstein - Primakoff transformation via the square roots they are expanded as a finite series in powers of the occupation numbers. This approximate second quantization method is applicable if the average values of the occupation numbers, or spin deviations are small. For J = ½ the expansion is inaccurate, Tyablikov[15].

$$\langle a_\ell^+ a_\ell \rangle \ll 2J \tag{3.20}$$

Expanding the Holstein - Primakoff square root we find:

$$\sqrt{1-\frac{a_\ell^+ a_\ell}{2J}} = 1 - \frac{1}{4J} a_\ell^+ a_\ell - \frac{1}{32J^2} a_\ell^+ a_\ell a_\ell^+ a_\ell - \cdots \tag{3.21}$$

and therefore the approximate transformation formulae turn out to be

$$J_l^z = J - a_l^+ a_l \tag{3.22}$$

$$J_l^+ \cong \sqrt{2J}\left(a_l - \frac{1}{4J} a_l^+ a_l a_l - \frac{1}{32J^2} a_l^+ a_l a_l^+ a_l a_l - \cdots\right) \tag{3.23}$$

$$J_l^- \cong \sqrt{2J}\left(a_l^+ - \frac{1}{4J} a_l^+ a_l^+ a_l - \frac{1}{32J^2} a_l^+ a_l^+ a_l a_l^+ a_l - \cdots\right) \tag{3.24}$$

It should be noted that the transformation is Hermitian because $(J^+)^+ = J^-$ and $(J^-)^+ = J^+$.

In the approximate second quantization method where the Holstein - Primakoff square root is expanded in powers of $a_l^+ a_l$ all higher order terms contribute to terms of lower order in the expansion using the commutation relation between Bose operators. A well ordering of the Holstein - Primakoff square root, which means that all a_l^+ operators come in front of all the a_l operators, involves a to the left commutation of all higher order terms.

It is possible to carry out the well ordering of the $\sqrt{1 - \frac{a_l^+ a_l}{2J}}$ expansion of the Holstein - Primakoff transformation. We use the following relations

$$\begin{aligned}(a_l^+ a_l)^n &= a_l^+ (a_l^+ a_l + 1)^{n-1} a_l \\ &= a_l^+ \sum_{p=0}^{n-1} \binom{n-1}{p} (a_l^+ a_l)^p \, a_l\end{aligned} \tag{3.25}$$

and

$$\sum_{p=1}^{n-1} \binom{n-1}{p} x^p = (1+x)^{n-1} - 1 \tag{3.26}$$

We find

$$\sqrt{1-\frac{a_l^+a_l}{2J}} = 1+\left\{\sqrt{1-\frac{1}{2J}}-1\right\}a_l^+a_l$$
$$+\left\{\frac{1}{2}\left(\sqrt{1-\frac{1}{J}}-1\right)-\left(\sqrt{1-\frac{1}{2J}}-1\right)\right\}a_l^+a_l^+a_la_l$$
$$+\cdots \tag{3.27}$$

This expansion is exact and shows the correction terms from all order in $1/J$. Now the angular momentum operators are tensor operators of rank one. To use the Holstein - Primakoff method to calculate in terms of Bose operators expressions of tensor operators of rank higher than one is very cumbersome. To overcome this we use later in this section a different method where we formally expand the Racah operators in a well ordered Bose operator series and require that the matrix elements between corresponding states are equal.

In the Bose language terms with two Bose operators describe non-interacting magnons and terms with more Bose operators describe interactions between the magnons. After the number of the Bose operators we talk of multiscattering processes, for which reason four Bose operators describe a two-magnon interaction.

The interaction between magnons divides into two parts: the kinematic and the dynamic interactions. The kinematic interaction is due to non- Bose properties of the operators which occur in the Hamiltonian, and is a consequence of spin statistics, namely that the maximum number of spin deviations that can occur at any atomic site in a many-particle system with angular momentum J is 2J. Take as an example spins of magnitude $\frac{1}{2}$ then clearly two spin deviations cannot reside at the same site, and the interaction that prevents this from occurring, the kinematic interaction, is a repulsive one. The dynamic interaction arises because it costs less energy for a spin to suffer a deviation if the spins with which it directly interacts have also undergone deviations from their fully aligned state; the dynamic interaction is attractive, Marshall and Lovesey[16]. The terminology of kinematic and dynamic interactions was introduced by Dyson[17] in his analysis of two spin-wave interactions in the Heisenberg ferromagnet. He showed that at low temperatures the kinematic interaction is small.

To avoid this difficulty when doing interacting magnon calculations we follow Dyson[17], who says that the operators for a real spin system may be associated, in some hypothetical space, with "ideal spin wave operators", which possess Bose properties. Nearly independent excitations are meaningful only at low temperatures when the probabilities of the processes, which are calculated by means of ideal spin waves, are equal to the probabilities of the processes of the real system. Under these considerations, we can obtain the Dyson - Maleev spin to Bose operator transformation, Tyablikov[15]

$$J_l^z = J - a_l^+ a_l \tag{3.28}$$

$$J_l^+ = \sqrt{2J}\left(1 - \frac{1}{2J} a_l^+ a_l\right) a_l \tag{3.29}$$

$$J_l^- = \sqrt{2J}\, a_l^+ \tag{3.30}$$

The creation and annihilation operators for Dysons ideal spin waves obey Bose commutation relationships. But now the transformation is no longer a Hermitian transformation as J_l^+ and J_l^- are not adjoint. Consider as a check the $[J_l^+, J_l^-]$ commutator

$$\begin{aligned}
[J_l^+, J_l^-] &= \left[\sqrt{2J}\left(1 - \frac{1}{2J} a_l^+ a_l\right) a_l, \sqrt{2J}\, a_l^+\right] \\
&= 2J - a_l^+ a_l - [a_l^+ a_l, a_l^+] a_l \\
&= 2(J - a_l^+ a_l) \\
&= 2 J_l^z
\end{aligned} \tag{3.31}$$

Later Oguchi[18] has shown that the Dyson - Maleev transformation is equivalent with the Holstein - Primakoff transformation.

3.3. Racah Operator Equivalents Expanded in Bose Operators

To calculate a well ordered Bose operator expansion of the Racah operators we formally expand the Racah operators in a well ordered series of Bose operators and require the matrix elements between corresponding states to be identical. In low temperature calculations we require correct matrix elements between the ground state and the first excited state. It turns out that it is only possible to match the matrix elements between two states exactly so in perturbation theories for higher temperatures an approximate matching of the matrix elements between the ground state and the excited states will be more appropriate. The well ordered expansion of the Racah operators is given by

$$\tilde{O}_{K,q} = \left(A^{K}_{q,0} + A^{K}_{q,1} a^{+}a + A^{K}_{q,2} a^{+}a^{+}aa + \cdots \right) a^{q} \qquad (3.32)$$

The coefficients are real and determined by matching the matrix elements in the following way

$$\langle J, J-n \,|\, \tilde{O}_{K,q} \,|\, J, J-(n+q) \rangle = \langle n | \left(A^{K}_{q,0} + A^{K}_{q,1} a^{+}a + A^{K}_{q,2} a^{+}a^{+}aa + \cdots \right) a^{q} | n+q \rangle \qquad (3.33)$$

Using formula (2.11) for the matrix element of a Racah operator and the formula for creation and annihilation operators acting on deviation eigenstates (3.18) and (3.19) we find.

$$(-1)^{n} \begin{pmatrix} J & K & J \\ -J+n & q & J-(n+q) \end{pmatrix} \langle J \| \tilde{O}_{K} \| J \rangle =$$
$$\sqrt{\frac{(n+q)!}{n!}} \left(A^{K}_{q,0} + n A^{K}_{q,1} + n(n-1) A^{K}_{q,2} + \cdots + n!\, A^{K}_{q,n} \right) \qquad (3.34)$$

From this formula we find the expansion coefficients

$$A^{K}_{q,n} = \sqrt{\frac{1}{n!\,(n+q)!}}\; (-1)^{n} \langle J \| \tilde{O}_{K} \| J \rangle \begin{pmatrix} J & K & J \\ -J+n & q & J-(n+q) \end{pmatrix}$$
$$- \left(\frac{1}{n!} A^{K}_{q,0} + \frac{1}{(n-1)!} A^{K}_{q,1} + \frac{1}{(n-2)!} A^{K}_{q,2} + \cdots + A^{K}_{q,n-1} \right) \qquad (3.35)$$

In appendix 3 it has been shown that for n = 0, n = 1 and n = 2 the coefficients turn out:

$$A^K_{q,0} = \frac{1}{\sqrt{q!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} \quad ; \quad n=0 \tag{3.36}$$

$$A^K_{q,1} = -\frac{1}{\sqrt{q!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} \cdot \left\{ 1 + \frac{1}{\sqrt{q+1}} \frac{\begin{pmatrix} J & K & J \\ -J+1 & q & J-(q+1) \end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix}} \right\}$$

$$n = 1 \tag{3.37}$$

$$A^K_{q,2} = \frac{1}{2} \frac{1}{\sqrt{q!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} \times \left\{ 1 + \frac{2}{\sqrt{q+1}} \frac{\begin{pmatrix} J & K & J \\ -J+1 & q & J-(q+1) \end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix}} + \frac{\sqrt{2}}{\sqrt{(q+1)(q+2)}} \frac{\begin{pmatrix} J & K & J \\ -J+2 & q & J-(q+2) \end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix}} \right\}$$

$$n = 2 \tag{3.38}$$

Instead of these cumbersome expressions for the expansion coefficients the following have been calculated in appendix 3

$$A^K_{q,0} = \frac{(-1)^q}{q!} \sqrt{\frac{(K+q)!}{2^q (K-q)!}} \frac{S_K}{\sqrt{S_q}} \quad ; \quad n=0 \tag{3.39}$$

$$A^K_{q,1} = -A^K_{q,0} \sqrt{\frac{S_q}{S_1 S_{q+1}}} \left\{ \frac{(K-q)(K+q+1)}{2(q+1)} + \sqrt{\frac{S_1 S_{q+1}}{S_q}} - \frac{S_{q+1}}{S_q} \right\}$$

$$n = 1 \tag{3.40}$$

$$A^{K}_{1,2} = -A^{K}_{1,0}\left\{\frac{(K-1)(K+2)}{4}\left[\frac{(K-2)(K+3)}{12}\frac{S_1}{S_2} + \frac{1}{\sqrt{S_2}}\left(1-\frac{\sqrt{S_1S_3}}{S_2}\right)\right] + \frac{1}{2}\left(1+\sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right\} \tag{3.41}$$

where the function S_K is also defined

$$S_K = \frac{1}{2^K}\frac{(2J)!}{(2J-K)!} = J(J-1/2)(J-1)(J-3/2)\cdots(J-\tfrac{K-1}{2}) \tag{3.42}$$

By means of these coefficient expressions and the general Bose operator expansion of the Racah operators they are calculated for odd values of K as well as even values of K up to K = 8, table (4). It should be noticed that all Racah operators are infinite expansions in Boseoperators included the operators $\tilde{O}_{1,0}\tilde{O}_{2,0}\cdots\tilde{O}_{8,0}$ The negative valued operators are found by means of (2.10). [illegible] operator expansions only terms with up to five Bose operators are written out because of the limited validity of the spin deviation representation. Further the Stevens operators expanded in Bose operators are calculated for all even values of K up to K = 8, table (5).

Finally in this section a comparison of the result of the two methods of expanding the angular momenta in Bose operators will be carried out. From table 1 and table 4 we find

$$\tilde{O}_{1,1} = -\frac{1}{\sqrt{2}}J^{+}_{\ell} = -\sqrt{S_1}\Big(a_\ell - \frac{1}{\sqrt{S_2}}\left(\sqrt{S_2}-\frac{S_2}{S_1}\right)a^{+}_{\ell}a_{\ell}a_{\ell} + \left[\frac{1}{2}\left(1+\sqrt{\frac{S_3}{S_1S_2}}\right)-\frac{\sqrt{S_2}}{S_1}\right]a^{+}_{\ell}a^{+}_{\ell}a_{\ell}a_{\ell}a_{\ell}+\cdots\Big) \tag{3.43}$$

Therefore we find for J^{+}, when we use

$$S_1 = J;\quad S_2 = J(J-1/2);\quad S_3 = J(J-1/2)(J-1)$$

$$J^{+}_{\ell} = \sqrt{2J}\Big[1+\left(\sqrt{1+\frac{1}{2J}}-1\right)a^{+}_{\ell}a_{\ell} + \left(\frac{1}{2}\left(\sqrt{1-\frac{1}{J}}-1\right)-\left(\sqrt{1-\frac{1}{2J}}-1\right)a^{+}_{\ell}a^{+}_{\ell}a_{\ell}a_{\ell}+\cdots\right)a_{\ell} \tag{3.44}$$

This expression calculated by matching matrix elements is exactly the same result as the Holstein - Primakoff method gives

4. THE TEMPERATURE DEPENDENCE OF THE SINGLE ION ANISOTROPY AND THE SINGLE ION MAGNETOSTRICTION

4.1. Single Ion Anisotropy and Single Ion Magnetostriction of a Ferromagnetic Crystal with Hexagonal Symmetry

The crystal field acting on a particular ion depends on the anisotropic distribution of the other ions in the lattice and on the conduction electrons. An additional contribution to the magneto crystalline anisotropy is caused by the magnetostrictive coupling between the magnetic moments of the ions and the crystal lattice. This magnetoelastic coupling accompanies the magnetic ordering in the crystal. In this section we want to calculate the temperature dependence of the single ion magneto crystalline anisotropy and the single ion magnetostriction of a ferromagnetic Bravais lattice with hexagonal symmetry. The magneto crystalline anisotropy of an unstrained hexagonal Bravais lattice in a c-axis representation is given by, Cooper, Elliott, Nettel and Suhl[19] and Goodings and Southern[20].

$$\mathcal{H}_{an} = \sum_i \left\{ B_2^0 O_2^0(c) + B_4^0 O_4^0(c) + B_6^0 O_6^0(c) + B_6^6 O_6^6(c) \right\}_i \tag{4.1}$$

The O_K^q (c) - operators are Stevens operators defined in (2.23) - (2.25) and the B_K^q - coefficients are the crystal field parameters after Elliott and Stevens[21].

For temperatures lower than the ordering temperature T_c, the single ion magneto elastic Hamiltonian of a hexagonal Bravais lattice is, Callen and Callen[22] and Danielsen[23].

$$\begin{aligned}
\mathcal{H}_{me} = -\sum_i \Big\{ & \left(B_{20}^{\alpha,1}\varepsilon^{\alpha,1} + B_{20}^{\alpha,2}\varepsilon^{\alpha,2}\right) O_2^0(c) + \left(B_{40}^{\alpha,1}\varepsilon^{\alpha,1} + B_{40}^{\alpha,2}\varepsilon^{\alpha,2}\right) O_4^0(c) \\
& + \left(B_{60}^{\alpha,1}\varepsilon^{\alpha,1} + B_{60}^{\alpha,2}\varepsilon^{\alpha,2}\right) O_6^0(c) + \left(B_{66}^{\alpha,1}\varepsilon^{\alpha,1} + B_{66}^{\alpha,2}\varepsilon^{\alpha,2}\right) O_6^6(c) \\
& + B_{22}^{\gamma}\left(\varepsilon_1^{\gamma} O_2^2(c) + \varepsilon_2^{\gamma} O_2^2(s)\right) + B_{42}^{\gamma}\left(\varepsilon_1^{\gamma} O_4^2(c) + \varepsilon_2^{\gamma} O_4^2(s)\right) \\
& + B_{62}^{\gamma}\left(\varepsilon_1^{\gamma} O_6^2(c) + \varepsilon_2^{\gamma} O_6^2(s)\right) + B_{44}^{\gamma}\left(\varepsilon_1^{\gamma} O_4^4(c) - \varepsilon_2^{\gamma} O_4^4(s)\right) \\
& + B_{64}^{\gamma}\left(\varepsilon_1^{\gamma} O_6^4(c) - \varepsilon_2^{\gamma} O_6^4(s)\right) + B_{21}^{\varepsilon}\left(\varepsilon_1^{\varepsilon} O_2^1(c) + \varepsilon_2^{\varepsilon} O_2^1(s)\right)
\end{aligned}$$

$$+ B_{41}^{\varepsilon}\left(\varepsilon_1^{\varepsilon} O_4^1(c) + \varepsilon_2^{\varepsilon} O_4^1(s)\right) + B_{61}^{\varepsilon}\left(\varepsilon_1^{\varepsilon} O_6^1(c) + \varepsilon_2^{\varepsilon} O_6^1(s)\right)$$

$$+ B_{65}^{\varepsilon}\left(\varepsilon_1^{\varepsilon} O_6^5(c) - \varepsilon_2^{\varepsilon} O_6^5(s)\right)\Big\}_i \qquad (4.2)$$

The magnetostriction has been expanded after the irreducible strains of the hcp-lattice, Callen and Callen[22]

$$\varepsilon^{\alpha,1} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

$$\varepsilon^{\alpha,2} = \frac{\sqrt{3}}{2}\left(\varepsilon_{zz} - \frac{1}{3}\varepsilon^{\alpha,1}\right)$$

$$\varepsilon_1^{\gamma} = \frac{1}{2}\left(\varepsilon_{xx} - \varepsilon_{yy}\right)$$

$$\varepsilon_2^{\gamma} = \varepsilon_{xy} \qquad (4.3)$$

$$\varepsilon_1^{\varepsilon} = \varepsilon_{yz}$$

$$\varepsilon_2^{\varepsilon} = \varepsilon_{xz}$$

$O_K^q(c)$ are the Stevens operators and the B'^s are magnetoelastic coupling constants. The elastic energy associated with the homogeneous strains is, Callen and Callen[22]

$$\mathcal{H}_{\ell} = \frac{1}{2} c_{11}^{\alpha}\left(\varepsilon^{\alpha,1}\right)^2 + c_{12}^{\alpha}\,\varepsilon^{\alpha,1}\varepsilon^{\alpha,2} + \frac{1}{2} c_{22}^{\alpha}\left(\varepsilon^{\alpha,2}\right)^2$$

$$+ \frac{1}{2} c^{\gamma}\left\{\left(\varepsilon_1^{\gamma}\right)^2 + \left(\varepsilon_2^{\gamma}\right)^2\right\} + \frac{1}{2} c^{\varepsilon}\left\{\left(\varepsilon_1^{\varepsilon}\right)^2 + \left(\varepsilon_2^{\varepsilon}\right)^2\right\} \qquad (4.4)$$

Omitting the non-homogeneous strains or phonon modes causes the elastic energy to be pure classical. The C'^s are the elastic constants of the group of the irreducible strains. They are related to the five independent Cartesian elastic constants by, Callen and Callen[22]

$$C_{11}^{\alpha} = \frac{1}{9}\left(2C_{11} + 2C_{12} + 4C_{13} + C_{33}\right)$$

$$C_{12}^{\alpha} = \frac{2}{3\sqrt{3}}\left(-C_{11} - C_{12} + C_{13} + C_{33}\right)$$

$$C_{22}^{\alpha} = \frac{2}{3}C_{11} + \frac{2}{3}C_{12} - \frac{8}{3}C_{13} + \frac{4}{3}C_{33} \tag{4.5}$$

$$C^{\gamma} = 2\left(C_{11} - C_{12}\right)$$

$$C^{\varepsilon} = 4C_{44}$$

Following Turov and Shavrov[24] and Cooper[25] we think of the magnetic moments of the spin wave precessing sufficiently fast that the magnetoelastic strains are unable to follow the precession. This is the frozen lattice model which implies a substitution of the equilibrium values for the irreducible strains.

Let ε^{Γ} be a shorthand notation for the irreducible strains of the hexagonal magnetic lattice. We separate the Hamiltonian in a strain dependent part $\mathcal{H}(\varepsilon^{\Gamma})$ and a strain independent part $\mathcal{H}_0$. We set up an expression for the free energy of the system and minimize the free energy with respect to the irreducible strains ε^{Γ} to find explicitly the irreducible equilibrium strains ε^{Γ}. The free energy is given by

$$\mathcal{F}(\varepsilon^{\Gamma}) = -k_B T \ln \mathrm{Tr}\left\{ e^{-(\mathcal{H}_0 + \mathcal{H}(\varepsilon^{\Gamma}))/k_B T} \right\} \tag{4.6}$$

The equilibrium strains are found by minimizing the free energy:

$$\frac{\partial \mathcal{F}(\varepsilon^{\Gamma})}{\partial \varepsilon^{\Gamma}} = -k_B T \frac{\mathrm{Tr}\left\{ -\frac{1}{k_B T} \frac{\partial \mathcal{H}(\varepsilon^{\Gamma})}{\partial \varepsilon^{\Gamma}} e^{-(\mathcal{H}_0 + \mathcal{H}(\varepsilon^{\Gamma}))/k_B T} \right\}}{\mathrm{Tr}\left\{ e^{-(\mathcal{H}_0 + \mathcal{H}(\varepsilon^{\Gamma}))/k_B T} \right\}}$$

or

$$\left\langle \frac{\partial \mathcal{H}(\varepsilon^{\Gamma})}{\partial \varepsilon^{\Gamma}} \right\rangle = 0 \tag{4.7}$$

It is not a simple task to differentiate inside a Tr-operation. The permissibility of doing so involves a knowledge of how the wave functions in the Tr-operation are influenzed by the differentiation procedure.

The actual calculation of the equilibrium strains is performed by means of (4.2) and (4.4). Expressed by the elastic constants, the magnetoelastic coupling constants and thermal mean values of the Stevens operators we have for the equilibrium strains (remember: a c-axis representation)

$$\bar{\varepsilon}^{\alpha,1} = \frac{1}{C_{11}^{\alpha}C_{22}^{\alpha} - (C_{12}^{\alpha})^2}\Big\{ (C_{22}^{\alpha} B_{20}^{\alpha,1} - C_{12}^{\alpha} B_{20}^{\alpha,2})\sum_i \langle O_2^0(c)\rangle_i + (C_{22}^{\alpha} B_{40}^{\alpha,1} - C_{12}^{\alpha} B_{40}^{\alpha,2})\sum_i \langle O_4^0(c)\rangle_i + (C_{22}^{\alpha} B_{60}^{\alpha,1} - C_{12}^{\alpha} B_{60}^{\alpha,2})\sum_i \langle O_6^0(c)\rangle_i + (C_{22}^{\alpha} B_{66}^{\alpha,1} - C_{12}^{\alpha} B_{66}^{\alpha,2})\sum_i \langle O_6^6(c)\rangle_i \Big\} \tag{4.8}$$

$$\bar{\varepsilon}^{\alpha,2} = \frac{1}{C_{11}^{\alpha}C_{22}^{\alpha} - (C_{12}^{\alpha})^2}\Big\{ (C_{11}^{\alpha} B_{20}^{\alpha,2} - C_{12}^{\alpha} B_{20}^{\alpha,1})\sum_i \langle O_2^0(c)\rangle_i + (C_{11}^{\alpha} B_{40}^{\alpha,2} - C_{12}^{\alpha} B_{40}^{\alpha,1})\sum_i \langle O_4^0(c)\rangle_i + (C_{11}^{\alpha} B_{60}^{\alpha,2} - C_{12}^{\alpha} B_{60}^{\alpha,1})\sum_i \langle O_6^0(c)\rangle_i + (C_{11}^{\alpha} B_{66}^{\alpha,2} - C_{12}^{\alpha} B_{66}^{\alpha,1})\sum_i \langle O_6^6(c)\rangle_i \Big\} \tag{4.9}$$

$$\bar{\varepsilon}_1^{\gamma} = \frac{1}{C^{\gamma}}\Big\{ B_{22}^{\gamma} \sum_i \langle O_2^2(c)\rangle_i + B_{42}^{\gamma} \sum_i \langle O_4^2(c)\rangle_i + B_{62}^{\gamma} \sum_i \langle O_6^2(c)\rangle_i + B_{44}^{\gamma} \sum_i \langle O_4^4(c)\rangle_i + B_{64}^{\gamma} \sum_i \langle O_6^4(c)\rangle_i \Big\} \tag{4.10}$$

$$\bar{\varepsilon}_2^{\gamma} = \frac{1}{c^{\gamma}}\Big\{ B_{22}^{\gamma}\sum_i \langle O_2^2(s)\rangle_i + B_{42}^{\gamma}\sum_i \langle O_4^2(s)\rangle_i + B_{62}^{\gamma}\sum_i \langle O_6^2(s)\rangle_i - B_{44}^{\gamma}\sum_i \langle O_4^4(s)\rangle_i - B_{64}^{\gamma}\sum_i \langle O_6^4(s)\rangle_i \Big\} \tag{4.11}$$

$$\bar{\varepsilon}_1^{\varepsilon} = \frac{1}{c^{\varepsilon}}\Big\{ B_{21}^{\varepsilon}\sum_i \langle O_2^1(c)\rangle_i + B_{41}^{\varepsilon}\sum_i \langle O_4^1(c)\rangle_i + B_{61}^{\varepsilon}\sum_i \langle O_6^1(c)\rangle_i + B_{65}^{\varepsilon}\sum_i \langle O_6^5(c)\rangle_i \Big\} \tag{4.12}$$

$$\bar{\varepsilon}_2^{\varepsilon} = \frac{1}{c^{\varepsilon}}\Big\{ B_{21}^{\varepsilon}\sum_i \langle O_2^1(s)\rangle_i + B_{41}^{\varepsilon}\sum_i \langle O_4^1(s)\rangle_i + B_{61}^{\varepsilon}\sum_i \langle O_6^1(s)\rangle_i - B_{65}^{\varepsilon}\sum_i \langle O_6^5(s)\rangle_i \Big\} \tag{4.13}$$

From the point of view that the magnetoelastic effect for $T < T_C$ causes a modification of the magnetocrystalline anisotropy we calculate the temperature dependence of the anisotropy. We see that the magneto striction causes a modification of the "unstrained" anisotropy terms as well as a generation of extra anisotropy terms. The temperature dependence of the unstrained anisotropy turns out to be, $T \le T_C$

$$\langle (\mathcal{H}_{an})_2^0 \rangle = \sum_i \Big\{ B_2^0(T_c) - B_{20}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{20}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \Big\} \langle O_2^0(c)\rangle_i \tag{4.14}$$

$$\langle (\mathcal{H}_{an})_4^0 \rangle = \sum_i \Big\{ B_4^0(T_c) - B_{40}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{40}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \Big\} \langle O_4^0(c)\rangle_i \tag{4.15}$$

$$\langle (\mathcal{H}_{an})_6^0 \rangle = \sum_i \Big\{ B_6^0(T_c) - B_{60}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{60}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \Big\} \langle O_6^0(c)\rangle_i \tag{4.16}$$

$$\langle (\mathcal{H}_{an})_6^6 \rangle = \sum_i \Big\{ B_6^6(T_c) - B_{66}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{66}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \Big\} \langle O_6^6(c)\rangle_i \tag{4.17}$$

or, in a shorthand notation defining effective temperature dependent crystal field parameters, $\mathcal{B}_q^K(T)$. The transition temperature T_c is used as a reference temperature.

$$\langle (\mathcal{H}_{an})_2^0 \rangle = \sum_i \mathcal{B}_2^0(T) \langle O_2^0(c) \rangle_i \tag{4.18}$$

$$\langle (\mathcal{H}_{an})_4^0 \rangle = \sum_i \mathcal{B}_4^0(T) \langle O_4^0(c) \rangle_i \tag{4.19}$$

$$\langle (\mathcal{H}_{an})_6^0 \rangle = \sum_i \mathcal{B}_6^0(T) \langle O_6^0(c) \rangle_i \tag{4.20}$$

$$\langle (\mathcal{H}_{an})_6^6 \rangle = \sum_i \mathcal{B}_6^6(T) \langle O_6^6(c) \rangle_i \tag{4.21}$$

from where we find for the effective temperature dependent crystal field parameters,

$$\mathcal{B}_2^0(T) = B_2^0(T_c) - B_{20}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{20}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \tag{4.22}$$

$$\mathcal{B}_4^0(T) = B_4^0(T_c) - B_{40}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{40}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \tag{4.23}$$

$$\mathcal{B}_6^0(T) = B_6^0(T_c) - B_{60}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{60}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \tag{4.24}$$

$$\mathcal{B}_6^6(T) = B_6^6(T_c) - B_{66}^{\alpha,1}(T)\,\bar{\varepsilon}^{\alpha,1}(T) - B_{66}^{\alpha,2}(T)\,\bar{\varepsilon}^{\alpha,2}(T) \tag{4.25}$$

The extra anisotropy terms are generated by the ε_1^γ, ε_2^γ, ε_1^ϵ and ε_2^ϵ strains. The temperature dependence of the anisotropy caused by these irreducible strains is

$$\begin{aligned}\langle (\mathcal{H}_{an})_{\bar{\varepsilon}_1^\gamma} \rangle = -\sum_i \bar{\varepsilon}_1^\gamma(T) \Big\{ & B_{22}^\gamma(T) \langle O_2^2(c) \rangle_i + B_{42}^\gamma(T) \langle O_4^2(c) \rangle_i \\ & + B_{62}^\gamma(T) \langle O_6^2(c) \rangle_i + B_{44}^\gamma(T) \langle O_4^4(c) \rangle_i \\ & + B_{64}^\gamma(T) \langle O_6^4(c) \rangle_i \Big\}\end{aligned} \tag{4.26}$$

$$\langle (\mathcal{H}_{an})_{\bar{\varepsilon}_2^\gamma} \rangle = -\sum_i \bar{\varepsilon}_2^\gamma(T) \Big\{ B_{22}^\gamma(T) \langle O_2^2(s) \rangle_i + B_{42}^\gamma(T) \langle O_4^2(s) \rangle_i + B_{62}^\gamma(T) \langle O_6^2(s) \rangle_i + B_{44}^\gamma(T) \langle O_4^4(s) \rangle_i + B_{64}^\gamma(T) \langle O_6^4(s) \rangle_i \Big\} \qquad (4.27)$$

$$\langle (\mathcal{H}_{an})_{\bar{\varepsilon}_1^\varepsilon} \rangle = -\sum_i \bar{\varepsilon}_1^\varepsilon(T) \Big\{ B_{21}^\varepsilon(T) \langle O_2^1(c) \rangle_i + B_{41}^\varepsilon(T) \langle O_4^1(c) \rangle_i + B_{61}^\varepsilon(T) \langle O_6^1(c) \rangle_i + B_{65}^\varepsilon(T) \langle O_6^5(c) \rangle_i \Big\} \qquad (4.28)$$

$$\langle (\mathcal{H}_{an})_{\bar{\varepsilon}_2^\varepsilon} \rangle = -\sum_i \bar{\varepsilon}_2^\varepsilon(T) \Big\{ B_{21}^\varepsilon(T) \langle O_2^1(s) \rangle_i + B_{41}^\varepsilon(T) \langle O_4^1(s) \rangle_i + B_{61}^\varepsilon(T) \langle O_6^1(s) \rangle_i + B_{65}^\varepsilon(T) \langle O_6^5(c) \rangle_i \Big\} \qquad (4.29)$$

The temperature dependence of the irreducible equilibrium strains is given by the formulae (4.8) - (4.13). At the critical transition temperature T_c we find for the temperature dependence of the anisotropy

$$\langle (\mathcal{H}_{an})_2^0 \rangle_{T=T_c} = \sum_i B_2^0(T_c) \langle O_2^0(c) \rangle_{i,T=T_c} \qquad (4.30)$$

$$\langle (\mathcal{H}_{an})_4^0 \rangle_{T=T_c} = \sum_i B_4^0(T_c) \langle O_4^0(c) \rangle_{i,T=T_c} \qquad (4.31)$$

$$\langle (\mathcal{H}_{an})_6^0 \rangle_{T=T_c} = \sum_i B_6^0(T_c) \langle O_6^0(c) \rangle_{i,T=T_c} \qquad (4.32)$$

$$\langle (\mathcal{H}_{an})_6^6 \rangle_{T=T_c} = \sum_i B_6^6(T_c) \langle O_6^6(c) \rangle_{i,T=T_c} \qquad (4.33)$$

The last expressions show explicitly the disappearence of the magnetoelastic coupling at $T = T_c$.

In the temperature region $T > T_c$ the magnetoelastic coupling is not effective as the magnetic moments are no longer ordered. On the other hand the normal thermal expansion is present. The temperature dependence of the anisotropy is therefore in this region determined by the temperature laws of the Stevens operators as as well the temperature variation of the crystal field parameters B_l^m. They depend on the lattice constants of the hexagonal lattice. In a point charge model calculation after Hutchings[9] we find this dependence to

$$B_l^m(r) \sim \frac{1}{r^{l+1}} \tag{4.34}$$

Taking the value of the lattice parameter r at $T = T_c$ as reference temperature we can expand the crystal field parameters from this value of the lattice parameter. For $T > T_c$ and to first order in the lattice parameter

$$B_l^m(T) \cong B_l^m(T_c) + \frac{\partial}{\partial r} B_l^m(T)_{T=T_c} \Delta r$$

but

$$B_l^m(r) \sim \frac{1}{r^{l+1}} \quad \text{for which reason}$$

$$\frac{\partial}{\partial r} B_l^m(r) \sim -(l+1) \frac{1}{r^{l+1}}$$

so

$$B_l^m(T) \cong B_l^m(T_c)\left(1-(l+1)\frac{\Delta r}{r}\right) \tag{4.35}$$

where Δr means the change in lattice parameter measured out from the lattice parameter value at $T = T_c$;

The temperature dependence of the anisotropy in the region $T > T_c$ therefore becomes:

$$\langle (\mathcal{H}_{an})_2^0 \rangle = \sum_i B_2^0(T_c)\left(1-3\frac{\Delta r}{r}\right)\langle O_2^0(c)\rangle_i \tag{4.36}$$

$$\langle (\mathcal{H}_{an})_4^0 \rangle = \sum_i B_4^0(T_c)\left(1-5\frac{\Delta r}{r}\right)\langle O_4^0(c)\rangle_i \tag{4.37}$$

$$\langle (\mathcal{H}_{an})_6^0 \rangle = \sum_i B_6^0(T_c)\left(1-7\frac{\Delta r}{r}\right)\langle O_6^0(c)\rangle_i \tag{4.38}$$

$$\langle (\mathcal{H}_{an})_6^6 \rangle = \sum_i B_6^6(T_c)\left(1-7\frac{\Delta r}{r}\right)\langle O_6^6(c)\rangle_i \tag{4.39}$$

4.2. Temperature Dependence of the Stevens Operators

To find the temperature laws of the single ion anisotropy and the single ion magnetostriction we must calculate the temperature dependence of the Stevens operators. This might be carried out by means of either a molecular field or a spin wave calculation. Using the Boseoperator expansions of the Stevens operators we here perform a low temperature spin wave calculation. In appendix 5 it is shown that the Hamiltonian of the magnetic system turns out to be

$$\mathcal{H} = \mathcal{E}_0 + \sum_q \left\{ \tfrac{1}{2} \mathcal{A}_q (a_q^+ a_q + a_q a_q^+) + \tfrac{1}{2} (\mathcal{B}_q a_q a_{-q} + \mathcal{B}_q^* a_{-q}^+ a_q^+) \right\} \tag{4.40}$$

As a consequence of including up to four Bose operators in the calculations (two-magnon interactions) the characteristic coefficients of the Hamiltonian are

$$\begin{aligned} \mathcal{A}_q &= A_q + \Delta A_q \\ \mathcal{B}_q &= B_q + \Delta B_q \\ \mathcal{E}_0 &= E_0 + \Delta E_0 \end{aligned} \tag{4.41}$$

Here the ΔE_0, ΔA_q and ΔB_q terms come from a treatment of these higher order terms in the Hartree-Fock approximation, which is a second order perturbation theory, while the E_0, A_g and B_q come from the non-interacting part of the Hamiltonian . In appendix 4 it is shown, using a method by Kowalska and Lindgård[26], how this Hamiltonian is diagonalized and brought to the form

$$\mathcal{H} = \mathcal{E}_0 + \sum_q \mathcal{E}_q \left(\hat{n}_q + \tfrac{1}{2} \right) \tag{4.42}$$

the familiar harmonic oscillator form
where

$$\varepsilon_q = \sqrt{A_q^2 - |B_q|^2} \tag{4.43}$$

is the dispersion relation of the interacting magnons and $\hat{n}_q$ is the number operator, $\hat{n}_q = F_q^+ F_q$. F_q^+ and F_g are creation operator and annihilation operator of the diagonal representation that are described by the eigenfunctions $|n_q\rangle$. The diagonal representation operators F_q^+ and F_q are connected with the Bose operators a_q^+, a_q through the relations

$$\begin{aligned} a_q &= \alpha_1 F_q + \alpha_2 F_{-q}^+ \\ a_{-q} &= \beta_1 F_{-q} + \beta_2 F_q^+ \end{aligned} \tag{4.44}$$

F_q, F_q^+, F_{-q} and F_{-q}^+ obey the Bose commutation relations

$$\begin{aligned} [F_q, F_q^+] &= 1 \\ [F_{-q}, F_{-q}^+] &= 1 \qquad \text{all other commutators being zero.} \end{aligned} \tag{4.45}$$

To calculate the temperature dependence of the single-ion anisotropy and the single-ion magnetostriction we set up a calculation of the temperature dependence of the Stevens operators summed over a Bravais lattice, so

$$\langle \sum_l O_K^q(\tfrac{c}{s}) \rangle = \frac{\mathrm{Tr}\{\sum_l O_K^q(\tfrac{c}{s})\, e^{-\mathcal{H}/k_B T}\}}{\mathrm{Tr}\{e^{-\mathcal{H}/k_B T}\}} \; ; \; q \neq 0 \tag{4.46}$$

and

$$\langle \sum_l O_K^0(c) \rangle = \frac{\mathrm{Tr}\{\sum_l O_K^0(c)\, e^{-\mathcal{H}/k_B T}\}}{\mathrm{Tr}\{e^{-\mathcal{H}/k_B T}\}} \; ; \; q = 0 \tag{4.47}$$

As a basis of these calculations we have performed the necessary Fourier transformations of the Bose operators in table 8. The non-interacting part of the Hamiltonian involves the following transformations

$$
\begin{aligned}
\sum_{\ell} a_{\ell}^{+} a_{\ell} &= \sum_{q} a_{q}^{+} a_{q} \\
\sum_{\ell} a_{\ell}^{+} a_{\ell}^{+} &= \sum_{q} a_{-q}^{+} a_{q}^{+} \\
\sum_{\ell} a_{\ell} a_{\ell} &= \sum_{q} a_{q} a_{-q}
\end{aligned}
\tag{4.48}
$$

The interacting part of the hamiltonian contains the four Bose operator expressions:

$$
\begin{aligned}
\sum_{\ell} a_{\ell}^{+} a_{\ell}^{+} a_{\ell}^{+} a_{\ell}^{+} &= \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^{+} a_{q_2}^{+} a_{-q_3}^{+} a_{-q_4}^{+} \, \delta_{q_1+q_2,\, q_3+q_4} \\
\sum_{\ell} a_{\ell}^{+} a_{\ell}^{+} a_{\ell}^{+} a_{\ell} &= \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^{+} a_{q_2}^{+} a_{-q_3}^{+} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4} \\
\sum_{\ell} a_{\ell}^{+} a_{\ell}^{+} a_{\ell} a_{\ell} &= \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^{+} a_{q_2}^{+} a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4} \\
\sum_{\ell} a_{\ell}^{+} a_{\ell} a_{\ell} a_{\ell} &= \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^{+} a_{-q_2} a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4} \\
\sum_{\ell} a_{\ell} a_{\ell} a_{\ell} a_{\ell} &= \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{-q_1} a_{-q_2} a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}
\end{aligned}
\tag{4.49}
$$

The thermal mean values of these two magnon interaction terms are decouple by use of the Hartree-Fock approximation giving:

$$\frac{1}{N}\sum_{\substack{q_1,q_2\\q_3q_4}} \delta_{q_1+q_2,q_3+q_4} \langle a^+_{q_1} a^+_{q_2} a_{q_3} a_{q_4}\rangle =$$
$$\frac{1}{N}\sum_{q_1,q_2}\left\{2\langle a^+_{q_1}a_{q_1}\rangle\langle a^+_{q_2}a_{q_2}\rangle + \langle a^+_{-q_1}a^+_{q_1}\rangle\langle a_{q_2}a_{-q_2}\rangle\right\} \tag{4.50}$$

$$\frac{1}{N}\sum_{\substack{q_1,q_2\\q_3q_4}} \delta_{q_1+q_2,q_3+q_4}\left[\langle a^+_{q_1}a^+_{q_2}a^+_{-q_3}a_{q_4}\rangle + \langle a^+_{q_1}a_{-q_2}a_{q_3}a_{q_4}\rangle\right] =$$
$$\frac{1}{N}\sum_{q_1q_2} 3\langle a^+_{q_1}a_{q_1}\rangle\left(\langle a^+_{-q_2}a^+_{q_2}\rangle + \langle a_{q_2}a_{-q_2}\rangle\right) \tag{4.51}$$

$$\frac{1}{N}\sum_{\substack{q_1q_2\\q_3q_4}} \delta_{q_1+q_2,q_3+q_4}\left[\langle a^+_{q_1}a^+_{q_2}a^+_{-q_3}a^+_{-q_4}\rangle + \langle a_{-q_1}a_{-q_2}a_{q_3}a_{q_4}\rangle\right] =$$
$$\frac{1}{N}\sum_{q_1q_2} 3\left(\langle a^+_{-q_1}a^+_{q_1}\rangle\langle a^+_{-q_2}a^+_{q_2}\rangle + \langle a_{q_1}a_{-q_1}\rangle\langle a_{q_2}a_{-q_2}\rangle\right) \tag{4.52}$$

We have only written out an even number of Bose operators as matrix elements of an odd number of Bose operators are zero. This means that the thermal mean values of Stevens operators $O_K^q\binom{c}{s}$, summed over a Bravais lattice, for q odd are zero. In a Bravais lattice the dispersion relation constant B_q is real (see app(4)), which implies the mean values of the Stevens operators O_K^q (s) with q even to be zero. Therefore the only mean values being different from zero are the following

$$\left\langle \sum_{\ell} O_K^q(c)\right\rangle \neq 0 \qquad \text{q even and } q \geq 0$$

The temperature dependences are of course different whether we do a non-interacting or a magnon-magnon interacting calculation. Below we distinguish between these two possibilities.

By means of the Bose operator expansions of the Stevens operators, given in table 5, a Fourier transformation and a Hartree-Fock approximation, we find, taking magnon-magnon interactions into account, the temperature dependence of the Stevens operators summed over a Bravais lattice.

$$\langle \sum_l O_2^0(l)\rangle = 2S_2 N\Big\{ 1 - \frac{3}{S_1 N}\sum_q \langle a_q^+ a_q\rangle$$

$$+ \frac{3}{2}\frac{1}{S_2 N^2}\sum_{q_1,q_2}\big(2\langle a_{q_1}^+ a_{q_1}\rangle\langle a_{q_2}^+ a_{q_2}\rangle + \langle a_{-q_1}^+ a_{q_1}^+\rangle\langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_2^2(l)\rangle = \sqrt{S_2}\, N\Big\{ \frac{1}{N}\sum_q \big(\langle a_{-q}^+ a_q^+\rangle + \langle a_q a_{-q}\rangle\big)$$

$$- \sqrt{\frac{S_2}{S_1 S_3}}\Big[\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big]\frac{3}{N^2}\sum_{q_1,q_2}\langle a_{q_1}^+ a_{q_1}\rangle\big(\langle a_{-q_2}^+ a_{q_2}^+\rangle + \langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_4^0(l)\rangle = 8S_4 N\Big\{ 1 - \frac{10}{S_1 N}\sum_q \langle a_q^+ a_q\rangle$$

$$+ \frac{45}{2}\frac{1}{S_2 N^2}\sum_{q_1,q_2}\big(2\langle a_{q_1}^+ a_{q_1}\rangle\langle a_{q_2}^+ a_{q_2}\rangle + \langle a_{-q_1}^+ a_{q_1}^+\rangle\langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_4^2(l)\rangle = 6\frac{S_4}{\sqrt{S_2}} N\Big\{ \frac{1}{N}\sum_q \big(\langle a_{-q}^+ a_q^+\rangle + \langle a_q a_{-q}\rangle\big)$$

$$- \sqrt{\frac{S_2}{S_1 S_3}}\Big[\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big]\frac{3}{N^2}\sum_{q_1,q_2}\langle a_{q_1}^+ a_{q_1}\rangle\big(\langle a_{-q_2}^+ a_{q_2}^+\rangle + \langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_4^4(l)\rangle = 6\sqrt{S_4}\;\frac{1}{N}\sum_{q_1,q_2}\big(\langle a_{-q_1}^+ a_{q_1}^+\rangle\langle a_{-q_2}^+ a_{q_2}^+\rangle + \langle a_{q_1} a_{-q_1}\rangle\langle a_{q_2} a_{-q_2}\rangle\big)$$

$$\langle \sum_l O_6^0(l)\rangle = 16 S_6 N\Big\{ 1 - \frac{21}{S_1 N}\sum_q \langle a_q^+ a_q\rangle$$

$$+ \frac{105}{S_2}\frac{1}{N^2}\sum_{q_1,q_2}\big(2\langle a_{q_1}^+ a_{q_1}\rangle\langle a_{q_2}^+ a_{q_2}\rangle + \langle a_{-q_1}^+ a_{q_1}^+\rangle\langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_6^2(l)\rangle = 16\frac{S_6}{\sqrt{S_2}} N\Big\{ \frac{1}{N}\sum_q \big(\langle a_{-q}^+ a_q^+\rangle + \langle a_q a_{-q}\rangle\big)$$

$$- \sqrt{\frac{S_2}{S_1 S_3}}\Big[6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big]\frac{3}{N^2}\sum_{q_1,q_2}\langle a_{q_1}^+ a_{q_1}\rangle\big(\langle a_{-q_2}^+ a_{q_2}^+\rangle + \langle a_{q_2} a_{-q_2}\rangle\big)\Big\}$$

$$\langle \sum_l O_6^4(l)\rangle = 60\frac{S_6}{\sqrt{S_4}}\;\frac{1}{N}\sum_{q_1,q_2}\big(\langle a_{-q_1}^+ a_{q_1}^+\rangle\langle a_{-q_2}^+ a_{q_2}^+\rangle + \langle a_{q_1} a_{-q_1}\rangle\langle a_{q_2} a_{-q_2}\rangle\big)$$

$$\langle \sum_{\ell} O_8^0(\ell) \rangle = 128\, S_8 N \Big\{ 1 - \frac{36}{S_1 N} \sum_q \langle a_q^+ a_q \rangle$$

$$+ \frac{315}{S_2} \frac{1}{N^2} \sum_{q_1 q_2} \left(2 \langle a_{q_1}^+ a_{q_1} \rangle \langle a_{q_2}^+ a_{q_2} \rangle + \langle a_{-q_1}^+ a_{q_1}^+ \rangle \langle a_{q_2} a_{-q_2} \rangle \right) \Big\}$$

$$\langle \sum_{\ell} O_8^2(\ell) \rangle = 32 \frac{S_8}{\sqrt{S_2}} N \Big\{ \frac{1}{N} \sum_q \left(\langle a_{-q}^+ a_q^+ \rangle + \langle a_q a_{-q} \rangle \right)$$

$$- \sqrt{\frac{S_2}{S_1 S_3}} \left[11 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right] \frac{3}{N^2} \sum_{q_1 q_2} \langle a_{q_1}^+ a_{q_1} \rangle \left(\langle a_{-q_2}^+ a_{q_2}^+ \rangle + \langle a_{q_2} a_{-q_2} \rangle \right) \Big\}$$

$$\langle \sum_{\ell} O_8^4(\ell) \rangle = 240 \frac{S_8}{\sqrt{S_4}} \frac{1}{N} \sum_{q_1 q_2} \left(\langle a_{-q_1}^+ a_{q_1}^+ \rangle \langle a_{-q_2}^+ a_{q_2}^+ \rangle + \langle a_{q_1} a_{-q_1} \rangle \langle a_{q_2} a_{-q_2} \rangle \right)$$

(4.53)

Two characteristic functions $\Delta M(T)$ and $b(T)$ are defined to bring the temperature laws of the Steven operators summed over a Bravais lattice on a more closed form. $\Delta M(T)$ is connected with the relative magnetization $m(T)$ through the relation

$$m(T) = \frac{M(T)}{M(0)} = 1 - \Delta M(T) \tag{4.54}$$

where $M(T)$ is the magnetization at temperature T and $M(o)$ the magnetization at $T = 0$. The $b(T)$ function accounts for the ellipticity or the non-circular spin pressesion about the direction of magnetization, therefore it is a result of the non-cylindrical anisotropy. $\Delta M(T)$ and $b(T)$ are defined through the relations

$$\Delta M(T) = \frac{1}{S_1 N} \sum_q \langle a_q^+ a_q \rangle$$

$$b(T) = \frac{1}{S_1 N} \sum_q \langle a_q a_{-q} \rangle \tag{4.55}$$

As already mentioned the B_q-coefficient of the diagonal energy expression is real for a Bravais lattice. This means that we have as well for a Bravais lattice

$$b(T) = \frac{1}{S_1 N} \sum_q \langle a_{-q}^+ a_q^+ \rangle \tag{4.55a}$$

Substituting the characteristic functions $\Delta M(T)$ and $b(T)$ we find:

$$\langle \sum_{l} O_2^0(c) \rangle = 2S_2 N \left\{ 1 - 3\Delta M(T) + \frac{3}{2}\frac{S_1^2}{S_2}\left(2\Delta M(T)^2 + b(T)^2\right) \right\}$$

$$\langle \sum_{l} O_2^2(c) \rangle = 2S_1 \sqrt{S_2}\, N\, b(T) \left\{ 1 - S_1 \sqrt{\frac{S_2}{S_1 S_3}} \left[\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right] 3\Delta M(T) \right\}$$

$$\langle \sum_{l} O_4^0(c) \rangle = 8S_4 N \left\{ 1 - 10\Delta M(T) + \frac{45}{2}\frac{S_1^2}{S_2}\left(2\Delta M(T)^2 + b(T)^2\right) \right\}$$

$$\langle \sum_{l} O_4^2(c) \rangle = 12 \frac{S_1 S_4}{\sqrt{S_2}} N\, b(T) \left\{ 1 - S_1 \sqrt{\frac{S_2}{S_1 S_3}} \left[\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right] 3\Delta M(T) \right\}$$

$$\langle \sum_{l} O_4^4(c) \rangle = 12\, S_1^2 \sqrt{S_4}\, N\, b(T)^2$$

$$\langle \sum_{l} O_6^0(c) \rangle = 16 S_6 N \left\{ 1 - 21\Delta M(T) + \frac{105}{S_2} S_1^2 \left(2\Delta M(T)^2 + b(T)^2\right) \right\}$$

$$\langle \sum_{l} O_6^2(c) \rangle = 32 \frac{S_1 S_6}{\sqrt{S_2}} N\, b(T) \left\{ 1 - S_1 \sqrt{\frac{S_2}{S_1 S_3}} \left[6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right] 3\Delta M(T) \right\}$$

$$\langle \sum_{l} O_6^4(c) \rangle = 120 \frac{S_1^2 S_6}{\sqrt{S_4}} N\, b(T)^2$$

$$\langle \sum_{l} O_8^0(c) \rangle = 128 S_8 N \left\{ 1 - 36\Delta M(T) + \frac{315}{S_2} S_1^2 \left(2\Delta M(T)^2 + b(T)^2\right) \right\}$$

$$\langle \sum_{l} O_8^2(c) \rangle = 64 \frac{S_1 S_8}{\sqrt{S_2}} N\, b(T) \left\{ 1 - S_1 \sqrt{\frac{S_2}{S_1 S_3}} \left[11 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right] 3\Delta M(T) \right\}$$

$$\langle \sum_{l} O_8^4(c) \rangle = 480 \frac{S_1^2 S_8}{\sqrt{S_4}} N\, b(T)^2 \qquad (4.56)$$

Stevens operators with $q > 4$ do not get contributions in a theory involving only two-magnon interactions treated in the Hartree-Fock approximation. These rather complicated expressions might be analysed in different ways making it possible to compare with simpler, but well-known theories.

In the infinite spin limit $J \to \infty$ the different J-dependent coefficients are examined.

$$1)\ \lim_{J\to\infty} \frac{S_1^2}{S_2} = 1$$

$$2)\ \lim_{J\to\infty} \left(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_2}{S_1} \right) = \frac{1}{2}$$

$$3)\ \lim_{J\to\infty} S_1 \sqrt{\frac{S_2}{S_1 S_3}} = 1$$

and the temperature laws then become

$$\left\langle \sum_l O_2^0(l) \right\rangle \cong 2 S_2 N \left\{ 1 - 3\Delta M(T) + 3\Delta M(T)^2 + \frac{3}{2} b(T)^2 \right\}$$

$$\left\langle \sum_l O_2^2(l) \right\rangle \cong 2 S_1 \sqrt{S_2}\, N\, b(T) \left(1 - \frac{3}{2} \Delta M(T) \right)$$

$$\left\langle \sum_l O_4^0(l) \right\rangle \cong 8 S_4 N \left\{ 1 - 10\Delta M(T) + 45\Delta M(T)^2 + \frac{45}{2} b(T)^2 \right\}$$

$$\left\langle \sum_l O_4^2(l) \right\rangle \cong 12 \frac{S_1 S_4}{\sqrt{S_2}} N\, b(T) \left(1 - \frac{17}{2} \Delta M(T) \right) \qquad (4.57)$$

$$\left\langle \sum_l O_4^4(l) \right\rangle \cong 12 S_1^2 \sqrt{S_4}\, N\, b(T)^2$$

$$\left\langle \sum_l O_6^0(l) \right\rangle \cong 16 S_6 N \left\{ 1 - 21\Delta M(T) + 210\Delta M(T)^2 + 105\, b(T)^2 \right\}$$

$$\left\langle \sum_l O_6^2(l) \right\rangle \cong 32 \frac{S_1 S_6}{\sqrt{S_2}} N\, b(T) \left(1 - \frac{39}{2} \Delta M(T) \right)$$

$$\left\langle \sum_l O_6^4(l) \right\rangle \cong 120 \frac{S_1^2 S_6}{\sqrt{S_4}} N\, b(T)^2$$

$$\left\langle \sum_l O_8^0(l) \right\rangle \cong 128 S_8 N \left\{ 1 - 36\Delta M(T) + 630\Delta M(T)^2 + 315\, b(T)^2 \right\}$$

$$\langle \sum_{\ell} O_8^2(c) \rangle \cong 64 \frac{S_1 S_8}{\sqrt{S_2}} N\, b(T) \left(1 - \frac{69}{2} \Delta M(T)\right)$$

$$\langle \sum_{\ell} O_8^4(c) \rangle \cong 480 \frac{S_1^2 S_8}{\sqrt{S_4}} N\, b(T)$$

To proceed we set up a Taylor series with $x = \Delta M(T)$ and use that $m(T) = 1 - \Delta M(T)$

$$(1-x)^{\alpha} = 1 - \alpha x + \frac{\alpha(\alpha-1)}{2!} x^2 - \cdots$$

$$\begin{aligned}
\alpha = 3: &\quad (1-\Delta M(T))^3 = 1 - 3\Delta M(T) + 3\Delta M(T)^2 - \cdots = m(T)^3 \\
\alpha = 10: &\quad (1-\Delta M(T))^{10} = 1 - 10\Delta M(T) + 45\Delta M(T)^2 - \cdots = m(T)^{10} \\
\alpha = 21: &\quad (1-\Delta M(T))^{21} = 1 - 21\Delta M(T) + 210\Delta M(T)^2 - \cdots = m(T)^{21} \\
\alpha = 36: &\quad (1-\Delta M(T))^{36} = 1 - 36\Delta M(T) + 630\Delta M(T)^2 - \cdots = m(T)^{36}
\end{aligned} \tag{4.58}$$

The temperature laws of the infinite spin limit are therefore only to second order in $\Delta M(T)$ and $b(T)$ by use of the Taylor expansions written as:

$q = 0$

$$\boxed{\langle \sum_{\ell} O_K^0(c) \rangle \cong \mathcal{B}_K^{(0)} S_K\, m(T)^{K(K+1)/2} \cdot \left(1 + b(T)^2\right)^{K(K+1)[K(K+1)-2]/16}} \tag{4.59}$$

explicitly for $K = 2, 4, 6$ and 8

$$\langle \sum_{\ell} O_2^0(c) \rangle \cong 2 S_2 N\, m(T)^3 \cdot \left(1 + b(T)^2\right)^{3/2}$$

$$\langle \sum_{\ell} O_4^0(c) \rangle \cong 8 S_4 N\, m(T)^{10} \cdot \left(1 + b(T)^2\right)^{45/2}$$

$$\langle \sum_{\ell} O_6^0(c) \rangle \cong 16 S_6 N\, m(T)^{21} \cdot \left(1 + b(T)^2\right)^{105}$$

$$\langle \sum_{\ell} O_8^0(c) \rangle \cong 128 S_8 N\, m(T)^{36} \cdot \left(1 + b(T)^2\right)^{315}$$

$q = 2$

$$\boxed{\left\langle \sum_{\ell} O_K^2(\ell) \right\rangle \cong \mathscr{C}_K^{(2)} S_K \frac{S_1}{\sqrt{S_2}}\, b(T)\, m(T)^{K(K+1)/2-\frac{3}{2}}} \tag{4.60}$$

explicitly for K = 2, 4, 6 and 8

$$\left\langle \sum_{\ell} O_2^2(\ell) \right\rangle \cong 2 S_1 \sqrt{S_2}\, N\, b(T)\, m(T)^{\frac{3}{2}}$$

$$\left\langle \sum_{\ell} O_4^2(\ell) \right\rangle \cong 12 \frac{S_1 S_4}{\sqrt{S_2}}\, N\, b(T)\, m(T)^{\frac{17}{2}}$$

$$\left\langle \sum_{\ell} O_6^2(\ell) \right\rangle \cong 32 \frac{S_1 S_6}{\sqrt{S_2}}\, N\, b(T)\, m(T)^{\frac{39}{2}}$$

$$\left\langle \sum_{\ell} O_8^2(\ell) \right\rangle \cong 64 \frac{S_1 S_8}{\sqrt{S_2}}\, N\, b(T)\, m(T)^{\frac{69}{2}}$$

$q = 4$

$$\boxed{\left\langle \sum_{\ell} O_K^4(\ell) \right\rangle \cong \mathscr{C}_K^{(4)} S_K \frac{S_1^2}{\sqrt{S_4}}\, b(T)^2} \tag{4.61}$$

explicitly for K = 4, 6 and 8

$$\left\langle \sum_{\ell} O_4^4(\ell) \right\rangle \cong 12\, S_1^2 \sqrt{S_4}\, N\, b(T)^2$$

$$\left\langle \sum_{\ell} O_6^4(\ell) \right\rangle \cong 120 \frac{S_1^2 S_6}{\sqrt{S_4}}\, N\, b(T)^2$$

$$\left\langle \sum_{\ell} O_8^4(\ell) \right\rangle \cong 480 \frac{S_1^2 S_8}{\sqrt{S_4}}\, N\, b(T)^2$$

<u>The b(T) = 0 limit</u>

If we put the parameter $b(T) = 0$ corresponding to circular spin precession or cylindrical anisotropy alone we find the temperature law of the Stevens operators with only $q = 0$ operators left.

$$\boxed{\langle \sum_{l} O_K^0(c) \rangle \cong \mathscr{C}_K^{(0)} S_K \, m(T)^{K(K+1)/2}} \tag{4.62}$$

This is nothing else than the well-known low temperature K(K + 1)/2 law, which has been calculated by many authors as the temperature law of the magneto crystalline anisotropy. This power law has been calculated by classical as well as quantum mechanical methods; see Callen and Callen[27] for a review. What the actual calculation in the infinite spin limit really does is to show that the second order term in this series comes exactly out.

The non-interacting limit

For finite spin values the calculation based on interacting magnons in a Hartree-Fock approximation explicitly sets up the different temperature laws of the Stevens operators $O_K^q(c)$ for $q = 0$, $q = 2$ and $q = 4$. But even a non-interacting calculation gives different temperature laws of the Stevens operators with $q = 0$, $q = 2$. For this non-interacting limit we find for finite spin values

$q=0$

$$\boxed{\langle \sum_{l} O_K^0(c) \rangle = \mathscr{C}_K^{(0)} S_K \, m(T)^{K(K+1)/2}} \tag{4.63}$$

$q=2$

$$\boxed{\langle \sum_{l} O_K^2(c) \rangle = \mathscr{C}_K^{(2)} S_K \frac{S_1}{\sqrt{S_2}} \, b(T)} \tag{4.64}$$

explicitly written out:

$q=0$

$$\langle \sum_{l} O_2^0(c) \rangle = 2 S_2 N \, m(T)^3$$

$$\langle \sum_{l} O_4^0(c) \rangle = 8 S_4 N \, m(T)^{10}$$

$$\langle \sum_{l} O_6^0(c) \rangle = 16 S_6 N \, m(T)^{21}$$

$$\langle \sum_{l} O_8^0(c) \rangle = 128 S_8 N \, m(T)^{36}$$

$q = 2$

$$\langle \sum_l O_2^2(c) \rangle = 2 S_1 \sqrt{S_2}\, N\, b(T)$$

$$\langle \sum_l O_4^2(c) \rangle = 12 \frac{S_1 S_4}{\sqrt{S_2}} N\, b(T)$$

$$\langle \sum_l O_6^2(c) \rangle = 32 \frac{S_1 S_6}{\sqrt{S_2}} N\, b(T)$$

$$\langle \sum_l O_8^2(c) \rangle = 64 \frac{S_1 S_8}{\sqrt{S_2}} N\, b(T) .$$

the q = 4 operators are zero in the non-interacting limit as they depend on b(T) to the second order.

On the basis of the calculated temperature laws of the Stevens operators we conclude that the $\bar{\varepsilon}_2^{\gamma}$, the $\bar{\varepsilon}_1^{\varepsilon}$, and the $\varepsilon_2^{\varepsilon}$ contributions to the magneto crystalline anisotropy are zero. Actually besides the unstrained anisotropy only the $\bar{\varepsilon}^{\alpha,1}$, $\bar{\varepsilon}^{\alpha,2}$ and $\bar{\varepsilon}_1^{\gamma}$ strains contribute to the magneto crystalline anisotropy. In the approximate infinite spin limit we find for the anisotropy and the magnetostriction, remembering the magnon-magnon interaction theory developed only holds for low temperatures ($T < T_c$)

$$\langle (\mathcal{H}_{an})_2^0 \rangle \cong \mathcal{B}_2^0(T)\, 2 S_2 N\, m(T)^3 \cdot (1 + b(T)^2)^{3/2}$$

$$\langle (\mathcal{H}_{an})_4^0 \rangle \cong \mathcal{B}_4^0(T)\, 8 S_4 N\, m(T)^{10} \cdot (1 + b(T)^2)^{45/2} \qquad (4.65)$$

$$\langle (\mathcal{H}_{an})_6^0 \rangle \cong \mathcal{B}_6^0(T)\, 16 S_6 N\, m(T)^{21} \cdot (1 + b(T)^2)^{105}$$

$$\langle (\mathcal{H}_{an})_6^6 \rangle \cong 0$$

The temperature dependence of the effective crystal field parameters given by (4.22) - (4.25) is expressed through the temperature variation of the strains $\varepsilon^{\alpha,1}$, $\bar{\varepsilon}^{\alpha,2}$ and $\bar{\varepsilon}_1^{\gamma}$

$$\bar{\varepsilon}^{\alpha,1}(T) = \frac{1}{C_{11}^{\alpha}C_{22}^{\alpha} - (C_{12}^{\alpha})^2}\Big\{(C_{22}^{\alpha}B_{20}^{\alpha,1}(T) - C_{12}^{\alpha}B_{20}^{\alpha,2}(T))\,2S_2 N m(T)^3 (1+b(T)^2)^{1}$$

$$+(C_{22}^{\alpha}B_{40}^{\alpha,1}(T) - C_{12}^{\alpha}B_{40}^{\alpha,2}(T))\,8S_4 N m(T)^{10}(1+b(T)^2)^{4}$$

$$+(C_{22}^{\alpha}B_{60}^{\alpha,1}(T) - C_{12}^{\alpha}B_{60}^{\alpha,2}(T))\,16S_6 N m(T)^{21}(1+b(T)^2)^{1}\Big\} \qquad (4.66)$$

$$\bar{\varepsilon}^{\alpha,2}(T) = \frac{1}{C_{11}^{\alpha}C_{22}^{\alpha} - (C_{12}^{\alpha})^2}\Big\{(C_{11}^{\alpha}B_{20}^{\alpha,2}(T) - C_{12}^{\alpha}B_{20}^{\alpha,1}(T))\,2S_2 N m(T)^3 (1+b(T)^2)^{3/2}$$

$$+(C_{11}^{\alpha}B_{40}^{\alpha,2}(T) - C_{12}^{\alpha}B_{40}^{\alpha,1}(T))\,8S_4 N m(T)^{10}(1+b(T)^2)^{15/2}$$

$$+(C_{11}^{\alpha}B_{60}^{\alpha,2}(T) - C_{12}^{\alpha}B_{60}^{\alpha,1}(T))\,16S_6 N m(T)^{21}(1+b(T)^2)^{105}\Big\} \qquad (4.67)$$

$$\bar{\varepsilon}_1^{\gamma}(T) = \frac{1}{C^{\gamma}}\Big\{ B_{22}^{\gamma}(T)\,2S_2 N b(T) m(T)^3 + B_{42}^{\gamma}(T)\,12\frac{S_1 S_4}{\sqrt{S_2}} N b(T) m(T)^{10}$$

$$+B_{62}^{\gamma}(T)\,32\frac{S_1 S_6}{\sqrt{S_2}} N b(T) m(T)^{21} + B_{44}^{\gamma}(T)\,12 S_1^2\sqrt{S_4}\, N b(T)^2$$

$$+B_{64}^{\gamma}(T)\,120\frac{S_1^2 S_6}{\sqrt{S_4}} N b(T)^2 \Big\} \qquad (4.68)$$

The only extra anisotropy term different from zero-generated by the ε_1^{γ} -strain is according to (4.26)

$$\langle(\mathcal{H}_{an})_{\bar{\varepsilon}_1^{\gamma}}\rangle = -\bar{\varepsilon}_1^{\gamma}(T)\Big\{B_{22}^{\gamma}(T)\,2S_1\sqrt{S_2}\, N b(T) m(T)^3$$

$$+B_{42}^{\gamma}(T)\,12\frac{S_1 S_4}{\sqrt{S_2}} N b(T) m(T)^{10}$$

$$+B_{62}^{\gamma}(T)\,32\frac{S_1 S_6}{\sqrt{S_2}} N b(T) m(T)^{21}$$

$$+B_{44}^{\gamma}(T)\,12 S_1^2\sqrt{S_4}\, N b(T)^2 + B_{64}^{\gamma}(T)\,120\frac{S_1^2 S_6}{\sqrt{S_4}} N b(T)^2\Big\}$$

The temperature dependence of $\bar{\varepsilon}_1^{\gamma}$ is given by (4.68). (4.69)

5. THE SPIN WAVE SPECTRUM OF THE HEAVY RARE EARTH METALS

5.1. Introduction

The spin wave excitations of the heavy rare earth metals are treated in this section. We want to calculate the temperature dependence of the spin wave dispersion relations. The temperature dependence of the spin wave energy gap is also treated in this section.

5.2. The Hamiltonian of the Heavy Rare Earth Metals

The crystal structure of the heavy rare earth metals is the hexagonal closed packed structure (h c p), of course with the c/a-ratio different from the ideal c/a-ratio of $\sqrt{8/3}$. The calculations are performed in a ferromagnetic structure and spin wave interactions are included to give renormalized expressions of the temperature dependence of the spin wave spectrum. The Hamiltonian consists of the isotopic exchange, the single-ion anisotropy, the single-ion magnetostriction, a term describing the effect of an externally applied magnetic field, and the elastic energy is also included.

The Hamiltonian therefore consists of the following terms

$$\mathcal{H} = \mathcal{H}_{ex} + \mathcal{H}_{an} + \mathcal{H}_{me} + \mathcal{H}_{Ze} + \mathcal{H}_{el} \tag{5.1}$$

The exchange interaction between the magnetic ions of the heavy rare earth metals is indirect. The direct overlap between the 4f-electrons, which carry the ionic moments, is negligible, but the 4f-electrons are coupled together quite strongly through the conduction electrons. It can be shown, see e.g. Mackintosh and Bjerrum Møller[28] that the indirect exchange interaction takes the isotropic Heisenberg form

$$\mathcal{H}_{ex} = \mathcal{H}_{ff} = -\sum_{l>l'} j(\bar{R}_l - \bar{R}_{l'})\, \bar{S}_l \cdot \bar{S}_{l'} \tag{5.2}$$

when $\underline{S}_l$ is the localized spin on the site $\underline{R}_l$ and $j(\underline{R}_l - \underline{R}_{l'})$ the exchange function that depends on the susceplibility of the conduction electrons. But the strong spin-orbit coupling in the 4f-shell of the rare earth metals causes $\underline{S}$ not to be a constant of motion. Projecting $\underline{S}$ on the total angular momentum J, μ_β is the Bohr Magneton and g is the Lande factor

$$\left.\begin{array}{l} \underline{J} = \underline{L} + \underline{S} \\ \underline{J} g \mu_B = \mu_B (\underline{L} + 2\underline{S}) \end{array}\right\} \Rightarrow \quad (g-1)\underline{J} = \underline{S} \tag{5.3}$$

we find

$$\begin{aligned} \mathcal{H}_{ex} &= -\sum_{l>l'} (g-1)^2 j(\bar{R}_l - \bar{R}_{l'})\, \bar{J}_l \cdot \bar{J}_{l'} \\ &= -\sum_{l>l'} \mathcal{J}(\bar{R}_l - \bar{R}_{l'})\, \bar{J}_l \cdot \bar{J}_{l'} \end{aligned} \tag{5.4}$$

where the exchange function now is

$$\mathcal{J}(\bar{R}_l - \bar{R}_{l'}) = (g-1)^2 j(\bar{R}_l - \bar{R}_{l'}) \tag{5.5}$$

It should be mentoned that the isotropic Heisenberg form (5.5) only provides as a first approximation to the exchange in the heavy rare earths a: it has been shown by H. B. Møller et al[29] that anisotropic exchange is important.

As the hexagonal closed packed structure consists of two interpenetratin sublattices the isotrop exchange takes the form

$$\begin{aligned} \mathcal{H}_{ex} = &-\sum_{l>l'} \mathcal{J}(\bar{R}_{ll'})\, \bar{J}_l \cdot \bar{J}_{l'} - \sum_{m>m'} \mathcal{J}(\bar{R}_{mm'})\, \bar{J}_m \cdot \bar{J}_{m'} \\ &-\sum_{l,m} \mathcal{J}'(\bar{R}_{lm})\, \bar{J}_l \cdot \bar{J}_m \end{aligned} \tag{5.6}$$

where the two first terms are intra sublattice exchange characterised by the exchange functions $\mathcal{J}(R_{ll'})$, $\mathcal{J}(R_{mm'})$, l and m being lattice sites in the two sublattices indexed l and m. The third term of the isotrop exchange is the inter sublattice exchange characterized by the inter sublattice exchange function $\mathcal{J}(R_{lm})$.

For a hexagonal lattice, we may write the Hamiltonian for the crystal field anisotropy in the c-representation in the form

$$\mathcal{H}_{an} = \sum_i \left\{ B_2^0 O_2^0(c) + B_4^0 O_4^0(c) + B_6^0 O_6^0(c) + B_6^6 O_6^6(c) \right\}_i \tag{5.7}$$

The crystal field acting on a particular ion, which is a result of the anisotropic distribution of the other ions and conduction electrons, produces a splitting of the 4f-levels. The minimization of this crystal field energy causes a preferential orientation of the magnetic moments, which may be viewed classically as resulting from the action of the crystalline electric field on the anisotropic 4f-charge distribution. The large spin-orbit coupling then ensures that the spin, as well as the orbital moment, follow the charge distribution. The $\mathcal{B}_K^q$-coefficients are the crystal field parameters defined by Elliott and Stevens[21]. A point charge calculation of the crystal field parameters has been done by Danielsen[23]. From group theory it can be shown that in the hcp -structure only B_2^0, B_4^0, B_6^0 and B_6^6 are non-zero. (In an ideal hcp-structure, $c/a = \sqrt{8/3}$ the B_2^0-parameter is zero). The $O_K^q(c)$ operators are the Stevens operators, defined in (2.23) - (2.25). In some of the heavy rare earths the axis of magnetization lies in the hexagonal or basal plan. This involves no problems of the isotropic exchange but for the anisotropy such a change in orientation of the quantization axis might be treated by a rotation through the specific Euler angles (α, β, γ) that transforms the axis of quantization (the c-axis) to the direction of magnetization. This rotation of the Stevens operators are done by use of the rotation of Racah operators (2.1) and the fact that the Stevens operators are linear combinations of Racah operators (2.23)-(2.25). Such rotations of Stevens operators have been treated in details by Danielsen and Lindgård[8].

On the basis of this work the general rotations of the Stevens operators have been calculated and written out in table 6. We shall hereafter refer to this table for all Stevens operator rotation problems.

Magnetic ordering may be accompanied by a magnetostrictive strain, which reduces the energy of the system by modifying the crystal fields. Such a magnetoelastic effect makes an additional contribution to the magnetic anisotropy. Thinking of the spin waves in the classical picture the precession of the moments in a spin wave is sufficiently fast for the magneto elastic strain to be unable to follow it; it therefore remains static. This is the frozen lattice model proposed by Turov and Sharov[24].

In addition to single-ion contributions to the magnetoelastic coupling a two-ion coupling may also be active. This effect has not together with the anisotropic exchange been treated in the actual case, as it requires a more elaborate theory of tensor operators including rotations of tensor operator products. The single-ion magnetoelastic Hamiltonian is here set up on the basis of the irreducible strains of the hcp-lattice and a group theoretical consideration of the symmetry of the hexagonal lattice done by Danielsen[23]. The irreducible strains of the hcp-lattice are given in (4.3).

$$\mathcal{H}_{me} = -\sum_i \Big\{ (B_{20}^{\alpha,1}\varepsilon^{\alpha,1} + B_{20}^{\alpha,2}\varepsilon^{\alpha,2}) O_2^0(c) + (B_{40}^{\alpha,1}\varepsilon^{\alpha,1} + B_{40}^{\alpha,2}\varepsilon^{\alpha,2}) O_4^0(c)$$

$$+ (B_{60}^{\alpha,1}\varepsilon^{\alpha,1} + B_{60}^{\alpha,2}\varepsilon^{\alpha,2}) O_6^0(c) + (B_{66}^{\alpha,1}\varepsilon^{\alpha,1} + B_{66}^{\alpha,2}\varepsilon^{\alpha,2}) O_6^6(c)$$

$$+ B_{22}^{\gamma}(\varepsilon_1^{\gamma} O_2^2(c) + \varepsilon_2^{\gamma} O_2^2(s)) + B_{42}^{\gamma}(\varepsilon_1^{\gamma} O_4^2(c) + \varepsilon_2^{\gamma} O_4^2(s))$$

$$+ B_{62}^{\gamma}(\varepsilon_1^{\gamma} O_6^2(c) + \varepsilon_2^{\gamma} O_6^2(s)) + B_{44}^{\gamma}(\varepsilon_1^{\gamma} O_4^4(c) - \varepsilon_2^{\gamma} O_4^4(s))$$

$$+ B_{64}^{\gamma}(\varepsilon_1^{\gamma} O_6^4(c) - \varepsilon_2^{\gamma} O_6^4(s)) + B_{21}^{\varepsilon}(\varepsilon_1^{\varepsilon} O_2^1(c) + \varepsilon_2^{\varepsilon} O_2^1(s))$$

$$+ B_{41}^{\varepsilon}(\varepsilon_1^{\varepsilon} O_4^1(c) + \varepsilon_2^{\varepsilon} O_4^1(s)) + B_{61}^{\varepsilon}(\varepsilon_1^{\varepsilon} O_6^1(c) + \varepsilon_2^{\varepsilon} O_6^1(s))$$

$$+ B_{65}^{\varepsilon}(\varepsilon_1^{\varepsilon} O_6^5(c) - \varepsilon_2^{\varepsilon} O_6^5(s)) \Big\}_i \tag{5.8}$$

The B's are phenomenological magnetoelastic coupling constants and the irreducible strains are taken as their equilibrium values because of the frozen lattice approximation. They have been calculated in section (4) while the coupling constants within the limitations of the point charge model of the crystal field have been calculated by Danielsen[23]. The effect of an external applied magnetic field H contributes with a term in the Hamiltonian

$$\mathcal{H}_{Zee} = -g\mu_0 \sum_{\ell} \underline{H}\cdot\underline{J}_{\ell} \tag{5.9}$$

where g is the Lande factor and μ_β the Bohr magneton. The elastic energy associated with the homogeneous strains is, Callen and Callen[22]

$$\mathcal{H}_{el} = \tfrac{1}{2} c_{11}^{\alpha}(\varepsilon^{\alpha,1})^2 + c_{12}^{\alpha}\varepsilon^{\alpha,1}\varepsilon^{\alpha,2} + \tfrac{1}{2} c_{22}^{\alpha}(\varepsilon^{\alpha,2})^2$$

$$+ \tfrac{1}{2} c^{\gamma}\big((\varepsilon_1^{\gamma})^2 + (\varepsilon_2^{\gamma})^2\big) + \tfrac{1}{2} c^{\varepsilon}\big((\varepsilon_1^{\varepsilon})^2 + (\varepsilon_2^{\varepsilon})^2\big) \tag{5.10}$$

The c's are the elastic constants which are related to the five independent Cartesian elastic constants given in (4.5)

5.3. The Temperature Dependence of the Spin Wave Spectrum of the Heavy Rare Earth Metals

The contribution from the different terms of the Hamiltonian to the spin wave dispersion relation has been treated in details in appendix 7. Taking into account magnon-magnon interactions the complete Hamiltonian is brought into the form

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 = \mathcal{H}_{ex} + \mathcal{H}_{an} + \mathcal{H}_{me} + \mathcal{H}_{Ze} \tag{5.11}$$

with

$$\mathcal{H}_0 = E_0 + \sum_K \Big\{ \tfrac{1}{2} A_K^a (a_K^+ a_K + a_K a_K^+) + \tfrac{1}{2} A_K^b (b_K^+ b_K + b_K b_K^+) + \tfrac{1}{2} (B_K^a a_K a_{-K} + B_K^{a*} a_{-K}^+ a_K^+) + \tfrac{1}{2} (B_K^b b_K b_{-K} + B_K^{b*} b_{-K}^+ b_K^+) + C_K a_K b_K^+ + C_K^* b_K a_K^+ \Big\} \tag{5.12}$$

and

$$\mathcal{H}_1 = \Delta E_0 + \sum_K \Big\{ \tfrac{1}{2} \Delta A_K^a (a_K^+ a_K + a_K a_K^+) + \tfrac{1}{2} \Delta A_K^b (b_K^+ b_K + b_K b_K^+) + \tfrac{1}{2} (\Delta B_K^a a_K a_{-K} + \Delta B_K^{a*} a_{-K}^+ a_K^+) + \tfrac{1}{2} (\Delta B_K^b b_K b_{-K} + \Delta B_K^{b*} b_{-K}^+ b_K^+) + \Delta C_K a_K b_K^+ + \Delta C_K^* b_K a_K^+ + \Delta D_K a_K b_{-K} + \Delta D_K^* b_{-K}^+ a_K^+ \Big\}$$

or in a closed form (5.13)

$$\mathcal{H} = \mathcal{E}_0 + \sum_K \Big\{ \tfrac{1}{2} \mathcal{A}_K^a (a_K^+ a_K + a_K a_K^+) + \tfrac{1}{2} \mathcal{A}_K^b (b_K^+ b_K + b_K b_K^+) + \tfrac{1}{2} (\mathcal{B}_K^a a_K a_{-K} + \mathcal{B}_K^{a*} a_{-K}^+ a_K^+) + \tfrac{1}{2} (\mathcal{B}_K^b b_K b_{-K} + \mathcal{B}_K^{b*} b_{-K}^+ b_K^+) + \mathcal{C}_K a_K b_K^+ + \mathcal{C}_K^* b_K a_K^+ + \Delta D_K a_K b_{-K} + \Delta D_K^* b_{-K}^+ a_K^+ \Big\} \tag{5.14}$$

a_K, a_K^+ are magnon operators of one sublattice indexed "a" and b_K, b_K^+ are magnon operators of the other sublattice indexed "b". The dispersion cons take up contributions from all terms of the Hamiltonian. They are given through the relations

$$\mathcal{E}_0 = E_0 + \Delta E_0 = \mathcal{E}_0(ex) + \mathcal{E}_0(an) + \mathcal{E}_0(me) + \mathcal{E}_0(Zee) \qquad (5.15)$$

$$\mathcal{A}_K^a = A_K^a + \Delta A_K^a = \mathcal{A}_K^a(ex) + \mathcal{A}_K^a(an) + \mathcal{A}_K^a(me) + \mathcal{A}_K^a(Zee) \qquad (5.16)$$

$$\mathcal{A}_K^b = A_K^b + \Delta A_K^b = \mathcal{A}_K^b(ex) + \mathcal{A}_K^b(an) + \mathcal{A}_K^b(me) + \mathcal{A}_K^b(Zee) \qquad (5.17)$$

$$\mathcal{B}_K^a = B_K^a + \Delta B_K^a = \mathcal{B}_K^a(ex) + \mathcal{B}_K^a(an) + \mathcal{B}_K^a(me) \qquad (5.18)$$

$$\mathcal{B}_K^{a*} = B_K^{a*} + \Delta B_K^{a*} = \mathcal{B}_K^{a*}(ex) + \mathcal{B}_K^{a*}(an) + \mathcal{B}_K^{a*}(me) \qquad (5.19)$$

$$\mathcal{B}_K^b = B_K^b + \Delta B_K^b = \mathcal{B}_K^b(ex) + \mathcal{B}_K^b(an) + \mathcal{B}_K^b(me) \qquad (5.20)$$

$$\mathcal{B}_K^{b*} = B_K^{b*} + \Delta B_K^{b*} = \mathcal{B}_K^{b*}(ex) + \mathcal{B}_K^{b*}(an) + \mathcal{B}_K^{b*}(me) \qquad (5.21)$$

$$\mathcal{C}_K = C_K + \Delta C_K = \mathcal{C}_K(ex) \qquad (5.22)$$

$$\mathcal{C}_K^* = C_K^* + \Delta C_K^* = \mathcal{C}_K^*(ex) \qquad (5.23)$$

$$\Delta \mathcal{D}_K = \Delta \mathcal{D}_K(ex) \qquad (5.24)$$

$$\Delta \mathcal{D}_K^* = \Delta \mathcal{D}_K^*(ex) \qquad (5.25)$$

The following relations hold for the dispersion constants, as the hcp-lattice built up from two interpenetrating Bravais sublattices.

$$A_K^a = A_K^b \tag{5.26}$$

$$B_K^a = B_K^b \tag{5.27}$$

$$C_K = C_K^* \tag{5.28}$$

$$\Delta D_K = \Delta D_K^* \tag{5.29}$$

The complete expressions of the dispersion constants are set up below. The renormalization has been treated in the Hartree Fock approximation by means of table 9. The structure is ferromagnetic with the moments lying in the hexagonal or basal plane. This is the structure of Tb and Dy.

The dispersion constants of the exchange

$$E_o(ex) = -N\left(\mathcal{J}(0)+\mathcal{J}'(0)\right) S_1(S_1+1) \tag{5.30}$$

$$\Delta E_o(ex) = \frac{1}{2N}\sum_{K_1}\left\{\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)+4(\sqrt{S_2}-S_1)\left(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2)\right)\times\right.$$
$$\left(\langle a_{K_1}^+ a_{K_1}\rangle + \langle b_{K_1}^+ b_{K_1}\rangle\right) +$$
$$\frac{1}{2N}\sum_{K_1 K_2}\left\{\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)+2(\sqrt{S_2}-S_1)\left(3\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2)\right)\times\right.$$
$$\left(\langle a_{K_1}^+ a_{K_1}\rangle\langle a_{K_2}^+ a_{K_2}\rangle + \langle b_{K_1}^+ b_{K_1}\rangle\langle b_{K_2}^+ b_{K_2}\rangle\right) -$$
$$2\sum_{K_2}(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)\langle a_{K_2}^+ b_{K_2}\rangle -$$
$$2\sum_{K_2}(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)^*\langle b_{K_2}^+ a_{K_2}\rangle -$$

$$
\begin{aligned}
&-\frac{1}{N}\sum_{K_1K_2}(S_1-\sqrt{S_2})\mathcal{J}'(\underline{K}_2)\Big(2\langle b^+_{K_1}b_{K_1}\rangle\langle a^+_{K_2}b_{K_2}\rangle+\langle b^+_{-K_2}a^+_{K_2}\rangle\langle b_{K_1}b_{-K_1}\rangle\Big)\\
&-\frac{1}{N}\sum_{K_1K_2}(S_1-\sqrt{S_2})\mathcal{J}'(\underline{K}_2)^*\Big(2\langle a^+_{K_1}a_{K_1}\rangle\langle b^+_{K_2}a_{K_2}\rangle+\langle a^+_{K_2}b^+_{K_2}\rangle\langle a_{K_1}a_{-K_1}\rangle\Big)\\
&-\frac{1}{N}\sum_{K_1K_2}(S_1-\sqrt{S_2})\Big(2\mathcal{J}'(\underline{K}_2)\langle a^+_{K_1}a_{K_1}\rangle\langle a^+_{K_2}b_{K_2}\rangle+\mathcal{J}'(\underline{K}_2)^*\langle a^+_{-K_1}a^+_{K_1}\rangle\langle a_{K_2}b_{-K_2}\rangle\\
&-\frac{1}{N}\sum_{K_1K_2}(S_1-\sqrt{S_2})\Big(2\mathcal{J}'(\underline{K}_2)^*\langle b^+_{K_1}b_{K_1}\rangle\langle b^+_{K_2}a_{K_2}\rangle+\mathcal{J}'(\underline{K}_2)^*\langle b^+_{-K_1}b^+_{K_1}\rangle\langle b_{K_2}a\\
&-\frac{1}{N}\sum_{K_1K_2}\mathcal{J}'(0)\langle a^+_{K_1}a_{K_1}\rangle\langle b^+_{K_2}b_{K_2}\rangle\\
&-\frac{1}{N}\sum_{K_1K_2}\mathcal{J}'(\underline{K}_1-\underline{K}_2)\Big(\langle a^+_{K_1}b_{K_1}\rangle\langle b^+_{K_2}a_{K_2}\rangle+\langle a^+_{K_1}b^+_{-K_1}\rangle\langle a_{K_2}b_{-K_2}\rangle\Big)\\
&-\frac{1}{2}\sum_{K_1}\mathcal{J}'(0)\Big(\langle a^+_{K_1}a_{K_1}\rangle+\langle b^+_{K_1}b_{K_1}\rangle\Big)\\
&-\frac{1}{2N}\sum_{K_1K_2}\Big\{2(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big)-\mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}\cdot\\
&\qquad\qquad\cdot\Big(\langle a^+_{K_1}a^+_{-K_1}\rangle\langle a_{K_2}a_{-K_2}\rangle+\langle b^+_{K_1}b^+_{K_1}\rangle\langle b_{K_2}b
\end{aligned}
\tag{5.31}
$$

$$
A^a_K(aa) = S_1\big(\mathcal{J}(0)-\mathcal{J}(\underline{K})+\mathcal{J}'(0)\big) \tag{5.32}
$$

$$
\begin{aligned}
\Delta A^a_{K_1}(aa) = \frac{1}{N}\sum_{K_2}\Big\{&\mathcal{J}(0)+\mathcal{J}(\underline{K}_1-\underline{K}_2)-4(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big)\langle a^+_{K_2}a_{K_2}\rangle\\
&+2(S_1-\sqrt{S_2})\Big(\mathcal{J}'(\underline{K}_2)^*\langle b^+_{K_2}a_{K_2}\rangle+\mathcal{J}'(\underline{K}_2)\langle a^+_{K_2}b_{K_2}\rangle\Big)\\
&+\mathcal{J}'(0)\langle b^+_{K_2}b_{K_2}\rangle\Big\}
\end{aligned}
\tag{5.33}
$$

$$A_{K}^{b}(xx) = S_1\left(\mathcal{J}(0) - \mathcal{J}(\underline{K}) + \mathcal{J}'(0)\right) \tag{5.34}$$

$$\begin{aligned}\Delta A_{K_1}^{b}(xx) = \frac{1}{N}\sum_{K_2}\Big\{&\left[\mathcal{J}(0) + \mathcal{J}(\underline{K}_1-\underline{K}_2) - 4(S_1-\sqrt{S_2})(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2))\right]\langle b_{K_2}^{+} b_{K_2}\rangle \\ &+ 2(S_1-\sqrt{S_2})\left(\mathcal{J}'(\underline{K}_2)^{*}\langle b_{K_2}^{+} a_{K_2}\rangle + \mathcal{J}'(\underline{K}_2)\langle a_{K_2}^{+} b_{K_2}\rangle\right. \\ &\left.+ \mathcal{J}'(0)\langle a_{K_2}^{+} a_{K_2}\rangle\right)\Big\}\end{aligned} \tag{5.35}$$

$$\begin{aligned}\Delta B_{K_2}^{a}(xx) = \frac{1}{N}\sum_{K_1}\Big\{&\left[2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\right]\langle a_{K_1}^{+} a_{-K_1}^{+}\rangle \\ &+ 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_1)^{*}\langle a_{K_1}^{+} b_{-K_1}^{+}\rangle\Big\}\end{aligned} \tag{5.36}$$

$$\begin{aligned}\Delta B_{K_2}^{a^+}(xx) = \frac{1}{N}\sum_{K_1}\Big\{&\left[2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\right]\langle a_{K_1} a_{-K_1}\rangle \\ &+ 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_1)\,\langle a_{K_1} b_{-K_1}\rangle\Big\}\end{aligned} \tag{5.37}$$

$$\begin{aligned}\Delta B_{K_2}^{b}(xx) = \frac{1}{N}\sum_{K_1}\Big\{&\left[2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\right]\langle b_{K_1}^{+} b_{-K_1}^{+}\rangle \\ &+ 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_1)\langle b_{-K_1}^{+} a_{K_1}^{+}\rangle\Big\}\end{aligned} \tag{5.38}$$

$$\begin{aligned}\Delta B_{K_2}^{b^+}(xx) = \frac{1}{N}\sum_{K_1}\Big\{&\left[2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\right]\langle b_{K_1} b_{-K_1}\rangle \\ &+ 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_1)^{*}\langle b_{-K_1} a_{K_1}\rangle\Big\}\end{aligned} \tag{5.39}$$

$$C_{\kappa}(ex) = -\mathcal{J}'(\underline{K})^{*} S_1 \tag{5.40}$$

$$\Delta C_{K_2}(ex) = \frac{1}{N}\sum_{K_1}\Big\{2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_2)^{*}\big(\langle a^{+}_{K_1}a_{K_1}\rangle + \langle b^{+}_{K_1}b_{K_1}\rangle\big) + \mathcal{J}'(\underline{K}_1-\underline{K}_2)\langle a^{+}_{K_1}b_{K_1}\rangle\Big\} \tag{5.41}$$

$$C^{*}_{K}(ex) = -\mathcal{J}'(\underline{K})S_1 \tag{5.42}$$

$$\Delta C^{*}_{K_2}(ex) = \frac{1}{N}\sum_{K_1}\Big\{2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_2)\big(\langle a^{+}_{K_1}a_{K_1}\rangle + \langle b^{+}_{K_1}b_{K_1}\rangle\big) + \mathcal{J}'(\underline{K}_1-\underline{K}_2)^{*}\langle b^{+}_{K_1}a_{K_1}\rangle\Big\} \tag{5.43}$$

$$\Delta D_{K_2}(ex) = \frac{1}{N}\sum_{K_1}\Big\{(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_2)^{*}\big(\langle a^{+}_{-K_1}a^{+}_{K_1}\rangle + \langle b^{+}_{-K_1}b^{+}_{K_1}\rangle\big) + \mathcal{J}'(\underline{K}_1-\underline{K}_2)\langle a^{+}_{K_1}b^{+}_{-K_1}\rangle\Big\} \tag{5.44}$$

$$\Delta D_{K_2}(ex)^{*} = \frac{1}{N}\sum_{K_1}\Big\{(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{K}_2)\big(\langle a_{K_1}a_{-K_1}\rangle + \langle b_{K_1}b_{-K_1}\rangle\big) + \mathcal{J}'(\underline{K}_1-\underline{K}_2)^{*}\langle a_{K_1}b_{-K_1}\rangle\Big\} \tag{5.45}$$

<u>The dispersion constants of the anisotropy</u> (two sublattices, a and b)

$$E_0(an) = N\Big\{-B_2^0 S_2\Big(1+\frac{3}{2S_1}\Big) + 3B_4^0 S_4\Big(1+\frac{5}{S_1}\Big) - (5B_6^0 - B_6^6\cos 6\alpha)S_6\Big(1+\frac{21}{2S_1}\Big)\Big\} \tag{5.46}$$

$$\Delta E_0(an) = \frac{1}{N}\Big(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_4}{S_2}\Big)\times$$
$$\times\Big\{2\sum_{K_1K_2}\big(\langle a^{+}_{K_1}a_{K_1}\rangle\langle a^{+}_{K_2}a_{K_2}\rangle + \langle b^{+}_{K_1}b_{K_1}\rangle\langle b^{+}_{K_2}b_{K_2}\rangle\big) - 2N\sum_{K_1}\big(\langle a^{+}_{K_1}a_{K_1}\rangle + \langle b^{+}_{K_1}b_{K_1}\rangle\big)\Big\}$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\tfrac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)-15B_4^0\tfrac{S_4}{\sqrt{S_2}}\Big(\tfrac{7}{3}+\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0+B_6^6\cos 6\alpha)\Big(6+\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)\Big)\times$$

$$\times\Big\{-\frac{3}{2}N\sum_{K_1}\big(\langle a_{K_1}^+a_{-K_1}^+\rangle+\langle b_{K_1}^+b_{-K_1}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle+\langle b_{K_1}b_{-K_1}\rangle\big)$$

$$-3\sum_{K_1K_2}\Big(\langle a_{K_2}^+a_{K_2}\rangle\big(\langle a_{K_1}^+a_{-K_1}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle\big)+\langle b_{K_2}^+b_{K_2}\rangle\big(\langle b_{K_1}^+b_{-K_1}^+\rangle+\langle b_{K_1}b_{-K_1}\rangle\big)\Big)\Big\}$$

$$+\frac{1}{N}\Big(\frac{35}{4}B_4^0\sqrt{S_4}-\frac{15}{4}(21B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\Big)\times$$

$$\Big\{-3\sum_{K_1K_2}\Big(\langle a_{K_1}^+a_{-K_1}^+\rangle\langle a_{K_2}^+a_{-K_2}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle\langle a_{K_2}a_{-K_2}\rangle$$

$$+\langle b_{K_1}^+b_{-K_1}^+\rangle\langle b_{K_2}^+b_{-K_2}^+\rangle+\langle b_{K_1}b_{-K_1}\rangle\langle b_{K_2}b_{-K_2}\rangle\Big)\Big\}$$

(5.47)

$$A_K^a(an)=3B_2^0\frac{S_2}{S_1}-30B_4^0\frac{S_4}{S_1}+21(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_1} \qquad (5.48)$$

$$\Delta A_K^a(an)=\Big(-\frac{3}{2}B_2^0+\frac{105}{2}B_4^0\frac{S_4}{S_2}-105(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_2}\Big)\frac{4}{N}\sum_{K_1}\langle a_{K_1}^+a_{K_1}\rangle$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\tfrac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)-15B_4^0\tfrac{S_4}{\sqrt{S_2}}\Big(\tfrac{7}{3}+\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0+B_6^6\cos 6\alpha)\Big(6+\sqrt{\tfrac{S_1S_3}{S_2}}-\tfrac{S_3}{S_2}\Big)\frac{S_6}{\sqrt{S_2}}\Big)\times$$

$$\times\,3\sum_{K_1}\big(\langle a_{K_1}^+a_{-K_1}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle\big) \qquad (5.49)$$

$$A_K^b(an)=3B_2^0\frac{S_2}{S_1}-30B_4^0\frac{S_4}{S_1}+21(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_1} \qquad (5.50)$$

$$\Delta A_k^b(an) = \left(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{S_2}\right)\frac{4}{N}\sum_{k_1}\langle b_{k_1}^+ b_{k_1}\rangle$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{3}{2}B_2^0\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right.$$

$$\left. + \frac{15}{2}(7B_6^0 + B_6^6\cos 6\alpha)\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\frac{S_6}{\sqrt{S_2}}\right) \times$$

$$\times 3\sum_{k_1}\left(\langle b_{k_1}^+ b_{-k_1}^+\rangle + \langle b_{k_1} b_{-k_1}\rangle\right) \qquad (5.51)$$

$$B_k^a(an) = -3B_2^0\sqrt{S_2} + 30B_4^0\frac{S_4}{\sqrt{S_2}} - 15(7B_6^0 + B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_2}} \qquad (5.52)$$

$$\Delta B_k^a(an) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{3}{2}B_2^0\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right.$$

$$\left. + \frac{15}{2}(7B_6^0 + B_6^6\cos 6\alpha)\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\frac{S_6}{\sqrt{S_2}}\right) \times$$

$$\times 6\sum_{k_1}\langle a_{k_1}^+ a_{k_1}\rangle$$

$$+\frac{1}{N}\left(\frac{35}{4}B_4^0\sqrt{S_4} - \frac{15}{4}(21B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\right) 12\sum_{k_1}\langle a_{k_1} a_{-k_1}\rangle$$

$$+\frac{1}{N}\left(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{S_2}\right)2\sum_{k_1}\langle a_{k_1}^+ a_{-k_1}^+\rangle \qquad (5.53)$$

$$\Delta B_k^{a^+}(an) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{3}{2}B_2^0\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right.$$

$$\left. + \frac{15}{2}(7B_6^0 + B_6^6\cos 6\alpha)\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right) \times$$

$$\times 6\sum_{k_1}\langle a_{k_1}^+ a_{k_1}\rangle$$

$$+\frac{1}{N}\left(\frac{35}{4}B_4^0\sqrt{S_4} - \frac{15}{4}(21B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\right) 12\sum_{k_1}\langle a_{k_1}^+ a_{-k_1}^+\rangle$$

$$+\frac{1}{N}\left(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{S_2}\right)2\sum_{k_1}\langle a_{k_1} a_{-k_1}\rangle \qquad (5.54)$$

$$B_K^b(an) = -3B_2^0\sqrt{S_2} + 30B_4^0\frac{S_4}{\sqrt{S_2}} - 15(7B_6^0 + B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_2}} \qquad (5.55)$$

$$\Delta B_K^b(an) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\frac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0 + B_6^6\cos 6\alpha)\Big(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big) \times$$

$$\times 6\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$

$$+\frac{1}{N}\Big(\frac{35}{4}B_4^0\sqrt{S_4} - \frac{15}{4}(21B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\Big)\,12\sum_{K_1}\langle b_{K_1} b_{-K_1}\rangle$$

$$+\frac{1}{N}\Big(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{S_2}\Big)\,2\sum_{K_1}\langle b_{K_1}^+ b_{-K_1}^+\rangle$$

(5.56)

$$\Delta B_K^{b^+}(an) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\frac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0 + B_6^6\cos 6\alpha)\Big(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\Big) \times$$

$$\times 6\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$

$$+\frac{1}{N}\Big(\frac{35}{4}B_4^0\sqrt{S_4} - \frac{15}{4}(21B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\Big)\,12\sum_{K_1}\langle b_{K_1}^+ b_{-K_1}^+\rangle$$

$$+\frac{1}{N}\Big(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105(5B_6^0 - B_6^6\cos 6\alpha)\frac{S_6}{S_2}\Big)\,2\sum_{K_1}\langle b_{K_1} b_{-K_1}\rangle$$

(5.57)

<u>The dispersion constants of the magnetostriction</u> (two sublattices, a and b)

$$E_0(me) = 2\mathcal{K}_2^0 S_2\Big(1 + \frac{3}{2S_1}\Big) + 8\mathcal{K}_4^0 S_4\Big(1 + \frac{5}{S_1}\Big) + 16\mathcal{K}_6^0 S_6\Big(1 + \frac{21}{2S_1}\Big)$$

(5.58)

$$\Delta E_0(me)=\frac{1}{N}\left(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\right)\cdot\Big\{-2N\sum_{K_1}\left(\langle a_{K_1}^+a_{K_1}\rangle+\langle b_{K_1}^+b_{K_1}\rangle\right)$$

$$-\sum_{K_1K_2}\Big(2\langle a_{K_1}^+a_{K_1}\rangle\langle a_{K_2}^+a_{K_2}\rangle+\langle a_{K_1}^+a_{-K_1}^+\rangle\langle a_{K_2}a_{-K_2}\rangle$$

$$+2\langle b_{K_1}^+b_{K_1}\rangle\langle b_{K_2}^+b_{K_2}\rangle+\langle b_{K_1}^+b_{-K_1}^+\rangle\langle b_{K_2}b_{-K_2}\rangle\Big)\Big\}$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\mathcal{K}_2^2\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)+\mathcal{K}_4^2\,6\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$

$$+\mathcal{K}_6^2\,16\frac{S_6}{\sqrt{S_2}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)\times$$

$$\times\Big\{3\sum_{K_1K_2}\Big(\langle a_{K_2}^+a_{K_2}\rangle\left(\langle a_{K_1}^+a_{-K_1}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle\right)+$$

$$\langle b_{K_2}^+b_{K_2}\rangle\left(\langle b_{K_1}^+b_{-K_1}^+\rangle+\langle b_{K_1}b_{-K_1}\rangle\right)\Big)+$$

$$\frac{3}{2}N\sum_{K_1}\left(\langle a_{K_1}^+a_{-K_1}^+\rangle+\langle a_{K_1}a_{-K_1}\rangle+\langle b_{K_1}^+b_{-K_1}^+\rangle+\langle b_{K_1}b_{-K_1}\rangle\right)\Big\}$$

$$-\frac{1}{N}\left(\mathcal{K}_4^4\,2\sqrt{S_4}+\mathcal{K}_6^4\,20\frac{S_6}{\sqrt{S_4}}\right)\times3\sum_{K_1K_2}\Big(\langle a_{K_1}^+a_{-K_1}^+\rangle\langle a_{K_2}^+a_{-K_2}^+\rangle$$

$$+\langle a_{K_1}a_{-K_1}\rangle\langle a_{K_2}a_{-K_2}\rangle+\langle b_{K_1}^+b_{-K_1}^+\rangle\langle b_{K_2}^+b_{-K_2}^+\rangle+\langle b_{K_1}b_{-K_1}\rangle\langle b_{K_2}b_{-K_2}\rangle\Big)$$

(5.59)

$$A_K^a(me)=-\left(6\mathcal{K}_2^0\frac{S_2}{S_1}+80\mathcal{K}_4^0\frac{S_4}{S_1}+336\mathcal{K}_6^0\frac{S_6}{S_1}\right)\qquad(5.60)$$

$$\Delta A_K^a(me)=\left(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\right)\frac{4}{N}\sum_{K_1}\langle a_{K_1}^+a_{K_1}\rangle$$

$$-\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\mathcal{K}_2^2\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)+\mathcal{K}_4^2\,6\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$

$$+\mathcal{K}_6^2\,16\frac{S_6}{\sqrt{S_2}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)3\sum_{K_1}\left(\langle a_{K_1}^+a_{K_1}^+\rangle+\langle a_{K_1}a_{K_1}\rangle\right)\qquad(5.61)$$

$$A_K^b(me) = -\left(6\mathcal{K}_2^0 \frac{S_2}{S_1} + 80\,\mathcal{K}_4^0 \frac{S_4}{S_1} + 336\,\mathcal{K}_6^0 \frac{S_6}{S_1}\right) \tag{5.62}$$

$$\begin{aligned}
\Delta A_K^b(me) = {} & \left(3\mathcal{K}_2^0 + 180\,\mathcal{K}_4^0 \frac{S_4}{S_2} + 840 \frac{S_6}{S_2} \mathcal{K}_6^0\right) \frac{4}{N} \sum_{K_1} \langle b_{K_1}^+ b_{K_1} \rangle \\
& - \frac{1}{N} \sqrt{\frac{S_2}{S_1 S_3}} \left(\mathcal{K}_2^2 \sqrt{S_2} \left(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} \left(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right. \\
& \left. + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}} \left(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right) 3 \sum_{K_1} \left(\langle b_{K_1}^+ b_{-K_1}^+ \rangle + \langle b_{K_1} b_{-K_1} \rangle \right)
\end{aligned} \tag{5.63}$$

$$B_K^a(me) = 2\left(\mathcal{K}_2^2 \sqrt{S_2} + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}}\right) \tag{5.64}$$

$$\begin{aligned}
\Delta B_K^a(me) = {} & -\frac{1}{N} \sqrt{\frac{S_2}{S_1 S_3}} \left(\mathcal{K}_2^2 \sqrt{S_2} \left(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} \left(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right. \\
& \left. + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}} \left(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right) 6 \sum_{K_1} \langle a_{K_1}^+ a_{K_1} \rangle \\
& + \frac{1}{N} \left(\mathcal{K}_4^4 2 \sqrt{S_4} + \mathcal{K}_6^4 20 \frac{S_6}{\sqrt{S_4}} \right) 12 \sum_{K_1} \langle a_{K_1} a_{-K_1} \rangle \\
& + \frac{1}{N} \left(3\mathcal{K}_2^0 + 180 \frac{S_4}{S_2} \mathcal{K}_4^0 + 840 \frac{S_6}{S_2} \mathcal{K}_6^0 \right) 2 \sum_{K_1} \langle a_{K_1}^+ a_{-K_1}^+ \rangle
\end{aligned} \tag{5.65}$$

$$\begin{aligned}
\Delta B_K^{a*}(me) = {} & -\frac{1}{N} \sqrt{\frac{S_2}{S_1 S_3}} \left(\mathcal{K}_2^2 \sqrt{S_2} \left(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} \left(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right. \\
& \left. + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}} \left(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right) 6 \sum_{K_1} \langle a_{K_1}^+ a_{K_1} \rangle \\
& + \frac{1}{N} \left(\mathcal{K}_4^4 2 \sqrt{S_4} + \mathcal{K}_6^4 20 \frac{S_6}{\sqrt{S_4}} \right) 12 \sum_{K_1} \langle a_{K_1}^+ a_{-K_1}^+ \rangle \\
& + \frac{1}{N} \left(3\mathcal{K}_2^0 + 180 \frac{S_4}{S_2} \mathcal{K}_4^0 + 840 \frac{S_6}{S_2} \mathcal{K}_6^0 \right) 2 \sum_{K_1} \langle a_{K_1} a_{K_1} \rangle
\end{aligned} \tag{5.66}$$

$$B_K^b(me) = 2\left(\mathcal{K}_2^2\sqrt{S_2}+\mathcal{K}_4^2 6\frac{S_4}{\sqrt{S_2}}+\mathcal{K}_6^2 16\frac{S_6}{\sqrt{S_2}}\right) \tag{5.67}$$

$$\Delta B_K^b(me) = -\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\mathcal{K}_2^2\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)+\mathcal{K}_4^2 6\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$
$$+\mathcal{K}_6^2 16\frac{S_6}{\sqrt{S_2}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)6\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$
$$+\frac{1}{N}\Big(\mathcal{K}_4^4 2\sqrt{S_4}+\mathcal{K}_6^4 20\frac{S_6}{\sqrt{S_4}}\Big)12\sum_{K_1}\langle b_{K_1} b_{-K_1}\rangle$$
$$+\frac{1}{N}\Big(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\Big)2\sum_{K_1}\langle b_{K_1}^+ b_{-K_1}^+\rangle \tag{5.68}$$

$$\Delta B_K^{b*}(me) = -\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\mathcal{K}_2^2\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)+\mathcal{K}_4^2 6\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$
$$+\mathcal{K}_6^2 16\frac{S_6}{\sqrt{S_2}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)6\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$
$$+\frac{1}{N}\Big(\mathcal{K}_4^4 2\sqrt{S_4}+\mathcal{K}_6^4 20\frac{S_6}{\sqrt{S_4}}\Big)12\sum_{K_1}\langle b_{K_1}^+ b_{-K_1}^+\rangle$$
$$+\frac{1}{N}\Big(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\Big)2\sum_{K_1}\langle b_{K_1} b_{-K_1}\rangle \tag{5.69}$$

$$\mathcal{K}_2^0 = \frac{1}{2}\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)-\frac{1}{2}B_{22}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) \tag{5.70}$$

$$\mathcal{K}_4^0 = -\frac{3}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)+\frac{1}{8}B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right)$$
$$-\frac{1}{8}B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.71}$$

$$\mathcal{H}_6^0 = \frac{5}{16}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{1}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{1}{16} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) + \frac{1}{16} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.72}$$

$$\mathcal{H}_2^2 = \frac{3}{2}\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{1}{2} B_{22}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) \tag{5.73}$$

$$\mathcal{H}_4^2 = -\frac{5}{2}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{1}{2} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right)$$
$$+ \frac{1}{2} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.74}$$

$$\mathcal{H}_4^4 = -\frac{35}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{7}{8} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right)$$
$$- \frac{1}{8} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.75}$$

$$\mathcal{H}_6^2 = \frac{105}{32}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{15}{32}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{17}{32} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) + \frac{5}{32} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.76}$$

$$\mathcal{H}_6^4 = \frac{63}{16}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{3}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{3}{16} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) - \frac{13}{16} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{5.77}$$

<u>The dispersion constants of the Zeeman term</u>

$$E_0(Zee) = -2\, g\mu_B H N \sin(\alpha+\delta)\left(S_1 + \frac{1}{2}\right) \tag{5.78}$$

$$A_K^a(Zee) = g\mu_B H \sin(\alpha+\delta) \tag{5.79}$$

$$A_K^b(Zee) = g\mu_B H \sin(\alpha+\delta) \tag{5.80}$$

The renormalized Hamiltonian is diagonalized using the method by Lindgård and Kowalska[26] giving a dispersion relation with two branches - an acoustical and an optical branch

$$\mathcal{H}_{diag} = \mathcal{E}_0 + \sum_K \left\{ \hbar\omega_K^{op}\left(F_K^+ F_K + \tfrac{1}{2}\right) + \hbar\omega_K^{ac}\left(G_K^+ G_K + \tfrac{1}{2}\right) \right\} \tag{5.81}$$

E_0 being the ground state energy, $\hbar\omega_K^{op}$ the optical excitation energies and $\hbar\omega_K^{ac}$ the acoustical excitation energies. $F_K^+ F_K$ and $G_K^+ G_K$ are the deviation or number operators of the optical and acoustical excitation modes. Expressed through the dispersion constants the excitation energies are

$$\hbar\omega_K^{op} = \left\{ (\mathcal{A}_K + |\mathcal{C}_K|) + |\mathcal{B}_K| \right\}^{1/2} \cdot \left\{ (\mathcal{A}_K + |\mathcal{C}_K|) - |\mathcal{B}_K| \right\}^{1/2} = \mathcal{E}_K^F \tag{5.82}$$

$$\hbar\omega_K^{ac} = \left\{ (\mathcal{A}_K - |\mathcal{C}_K|) + |\mathcal{B}_K| \right\}^{1/2} \cdot \left\{ (\mathcal{A}_K - |\mathcal{C}_K|) - |\mathcal{B}_K| \right\}^{1/2} = \mathcal{E}_K^G \tag{5.83}$$

To proceed in finding the temperature dependence of the dispersion relation the following thermal mean values appearing in the renormalized dispersion constants are to be calculated

$$\langle a_K^+ a_K \rangle, \ \langle b_K^+ b_K \rangle, \ \langle a_K a_{-K} \rangle, \ \langle a_{-K}^+ a_K^+ \rangle,$$

$$\langle b_K b_{-K} \rangle, \ \langle b_{-K}^+ b_K^+ \rangle, \ \langle a_K b_K^+ \rangle, \ \langle b_K a_K^+ \rangle,$$

$$\langle a_K b_{-K} \rangle, \ \langle b_{-K}^+ a_K^+ \rangle$$

As an example

$$\langle a_K^+ a_K \rangle = \frac{Tr\left\{ a_K^+ a_K \, e^{-\mathcal{H}_{diag}/k_0 T} \right\}}{Tr\left\{ e^{-\mathcal{H}_{diag}/k_0 T} \right\}}$$
$$= \sum_{F,G} \frac{\sum_{n_K} \langle n_K^{F,G} | a_K^+ a_K | n_K^{F,G} \rangle \, e^{-\mathcal{E}_K^{F,G}/k_0 T}}{\sum_{n_K} e^{-\mathcal{E}_K^{F,G}/k_0 T}} \tag{5.84}$$

$|n_K^{FG}\rangle$ are the eigenfunctions of the optical modes and the accoustical modes and $E_K^{F,G}$ the corresponding eigenvalues.

In appendix (8) all the thermal mean values have been calculated to:

$$\langle a_K^+ a_K\rangle = \frac{A_K+|C_K|}{2\,\varepsilon_K^F}\langle n_K^F\rangle + \frac{A_K-|C_K|}{2\,\varepsilon_K^G}\langle n_K^G\rangle + \frac{A_K+|C_K|}{4\,\varepsilon_K^F} + \frac{A_K-|C_K|}{4\,\varepsilon_K^G} - \frac{1}{2} \tag{5.85}$$

$$\langle b_K^+ b_K\rangle = \frac{C_K C_K^*}{|C_K|^2}\langle a_K^+ a_K\rangle \tag{5.86}$$

$$\langle a_{-K}^+ a_K^+\rangle = -\left(\frac{B_K}{2\varepsilon_K^F}\langle n_K^F\rangle + \frac{B_K}{2\varepsilon_K^G}\langle n_K^G\rangle + \frac{B_K}{4}\left(\frac{1}{\varepsilon_K^F}+\frac{1}{\varepsilon_K^G}\right)\right) \tag{5.87}$$

$$\langle a_K a_{-K}\rangle = -\left(\frac{B_K^*}{2\varepsilon_K^F}\langle n_K^F\rangle + \frac{B_K^*}{2\varepsilon_K^G}\langle n_K^G\rangle + \frac{B_K^*}{4}\left(\frac{1}{\varepsilon_K^F}+\frac{1}{\varepsilon_K^G}\right)\right) \tag{5.88}$$

$$\langle b_{-K}^+ b_K^+\rangle = \frac{C_K C_K^*}{|C_K|^2}\langle a_{-K}^+ a_K^+\rangle \tag{5.89}$$

$$\langle b_K b_{-K}\rangle = \frac{C_K C_K^*}{|C_K|^2}\langle a_K a_{-K}\rangle \tag{5.90}$$

$$\langle a_K b_K^+\rangle = \frac{C_K^*}{|C_K|}\left\{\frac{A_K+|C_K|}{2\varepsilon_K^F}\langle n_K^F\rangle - \frac{A_K-|C_K|}{2\varepsilon_K^G}\langle n_K^G\rangle + \frac{A_K+|C_K|}{4\varepsilon_K^F} - \frac{A_K-|C_K|}{4\varepsilon_K^G}\right\} \tag{5.91}$$

$$\langle b_K a_K^+\rangle = \frac{C_K}{|C_K|}\left\{\frac{A_K+|C_K|}{2\varepsilon_K^F}\langle n_K^F\rangle - \frac{A_K-|C_K|}{2\varepsilon_K^G}\langle n_K^G\rangle + \frac{A_K+|C_K|}{4\varepsilon_K^F} - \frac{A_K-|C_K|}{4\varepsilon_K^G}\right\} \tag{5.92}$$

$$\langle a_K b_{-K} \rangle = \frac{C_K^*}{|C_K|} \left\{ -\frac{B_K^*}{2E_K^F} \langle n_K^F \rangle + \frac{B_K^*}{2E_K^G} \langle n_K^G \rangle + \frac{B_K^*}{4} \left(\frac{1}{E_K^F} - \frac{1}{E_K^G} \right) \right\} \tag{5.93}$$

$$\langle b_{-K}^+ a_K^+ \rangle = \frac{C_K}{|C_K|} \left\{ -\frac{B_K}{2E_K^F} \langle n_K^F \rangle + \frac{B_K}{2E_K^G} \langle n_K^G \rangle + \frac{B_K}{4} \left(\frac{1}{E_K^G} - \frac{1}{E_K^F} \right) \right\} \tag{5.94}$$

where

$$\langle n_K^F \rangle = \frac{1}{e^{E_K^F/k_B T} - 1} \tag{5.95}$$

$$\langle n_K^G \rangle = \frac{1}{e^{E_K^G/k_B T} - 1} \tag{5.96}$$

are the Bose statistic factors, that must be calculated self consistent by means of the renormalized energies $E_K^{F,G}$ of the optical and acoustical branches.

As a check of the thermal mean values we symbolically compute them in "the Bravais lattice" limit which means $C_K = 0$ (no interlattice exchange) and $E_K^F = E_K^G = E_K \Rightarrow \langle n_K^F \rangle = \langle n_K^G \rangle$
In this limit we find

$$\langle b_K^+ b_K \rangle = \langle b_{-K}^+ b_K^+ \rangle = \langle b_K b_{-K} \rangle = \langle a_K b_K^+ \rangle = 0$$

$$\langle b_K a_K^+ \rangle = \langle a_K b_{-K} \rangle = \langle b_{-K}^+ a_K^+ \rangle = 0 \tag{5.97}$$

and

$$\langle a_K^+ a_K \rangle = \frac{A_K}{E_K} \left(\langle n_K \rangle + \frac{1}{2} \right) - \frac{1}{2} \tag{5.98}$$

$$\langle a_{-K}^+ a_K^+ \rangle = -\frac{B_K}{E_K} \left(\langle n_K \rangle + \frac{1}{2} \right) \tag{5.99}$$

$$\langle a_K a_{-K} \rangle = -\frac{B_K^*}{E_K} \left(\langle n_K \rangle + \frac{1}{2} \right) \tag{5.100}$$

A comparison with the formulae (A4.16) - (A4.18) shows the correspondence between the two set of calculations: In section 4 two characteristic functions were enough to describe the temperature variation of the single-ion anisotropy. A natural extension in connexion with the temperature dependence of the spin-wave spectrum is the following set of characteristic functions.

$$\Delta M(T)_a = \frac{1}{S_1 N} \sum_K \langle a_K^+ a_K \rangle \tag{5.101}$$

$$\Delta M(T)_b = \frac{1}{S_1 N} \sum_K \langle b_K^+ b_K \rangle \tag{5.102}$$

$$\ell(T)_a = \frac{1}{S_1 N} \sum_K \langle a_K a_{-K} \rangle \tag{5.103}$$

$$\ell(T)_a^* = \frac{1}{S_1 N} \sum_K \langle a_{-K}^+ a_K^+ \rangle \tag{5.104}$$

$$\ell(T)_b = \frac{1}{S_1 N} \sum_K \langle b_K b_{-K} \rangle \tag{5.105}$$

$$\ell(T)_b^* = \frac{1}{S_1 N} \sum_K \langle b_{-K}^+ b_K^+ \rangle \tag{5.106}$$

In proportion to sectior 4 we have here because the hcp-lattice is non Bravais that

$$\ell(T)_{a,b} \neq \ell(T)_{a,b}^* \tag{5.107}$$

Besides these characteristic functions we define some intra sublattice functions, namely

$$c(T) = \frac{1}{S_1 N} \sum_K \langle a_K b_K^+ \rangle \tag{5.108}$$

$$c(T)^* = \frac{1}{S_1 N} \sum_K \langle b_K a_K^+ \rangle \tag{5.109}$$

$$d(T) = \frac{1}{S_1 N} \sum_{k} \langle a_k b_{-k} \rangle \tag{5.110}$$

$$d(T)^* = \frac{1}{S_1 N} \sum_{k} \langle b_{-k}^+ a_k^+ \rangle \tag{5.111}$$

By means of these characteristic functions we express the temperature variation of the *renormalized dispersion constants*. Putting those into the formulae (5.82) and (5.83) we have calculated the temperature dependence of the spin wave spectrum.

5.4. The Temperature Dependence of the Spin Wave Energy Gap of the Heavy Rare Earth Metals

The anisotropy forces of the heavy rare earth metals cause the acoustic dispersion relation not to approach zero in the limit $q \to 0$, the long wavelength limit. From the expression of the acoustic excitation energies (5.83) we find the energy gap

$$\Delta(T)^2 = \mathcal{A}_0(T)^2 - \mathcal{B}_0(T)^2 \tag{5.112}$$

As the dispersion constants have been calculated under influenze of magnon magnon interactions in appendix 7 the energy gap is temperature dependent. Based on the detailed formulae in appendix 7 we set up the following relations for the dispersion constants

$$\begin{aligned} \mathcal{A}_0(T) + \mathcal{B}_0(T) = \; & \mathcal{A}_0(0) + \mathcal{B}_0(0) \\ & + f_M(B_l^m, \mathcal{K}_l^m, S_l)^+ \Delta M(T) \\ & + f_\ell(B_l^m, \mathcal{K}_l^m, S_l)^+ \ell(T) \end{aligned} \tag{5.113}$$

and

$$\mathcal{A}_0(T)-\mathcal{B}_0(T) = \mathcal{A}_0(0)-\mathcal{B}_0(0) + f_M(B_\ell^m,\mathcal{K}_\ell^m,S_\ell)^- \Delta M(T) + f_b(B_\ell^m,\mathcal{K}_\ell^m,S_\ell)^- b(T) \tag{5.114}$$

Here $\Delta M(T)$ and $b(T)$ are characteristic functions defined as in section 4. The *functions* $f_M^{\pm}$ and $f_b^{\pm}$ contain contributions from single ion anisotropy as well as from single ion magnetostriction. Explicitely written we find for $f_M^{\pm}$

$$\begin{aligned} f_M(B_\ell^m,\mathcal{K}_\ell^m,S_\ell)^{\pm} = 4S_1\Big\{ & -\tfrac{3}{2}B_2^0\Big(1\mp\frac{3S_2}{2\sqrt{S_1S_3}}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big) \\ & +\frac{135}{2}B_4^0\Big(1\mp\frac{1}{3}\frac{S_2}{\sqrt{S_1S_3}}\Big(\frac{2}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)\frac{S_4}{S_2} \\ & -525B_6^0\Big(1\mp\frac{2}{20}\frac{S_2}{\sqrt{S_1S_3}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)\frac{S_6}{S_2} \\ & +105B_6^6\cos 6\alpha\Big(1\pm\frac{1}{28}\frac{S_2}{\sqrt{S_1S_3}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big)\frac{S_6}{S_2} \\ & +3\Big(\mathcal{K}_2^0\mp\frac{S_2}{2\sqrt{S_1S_3}}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\mathcal{K}_2^2\Big) \\ & +180\Big(\mathcal{K}_4^0\mp\frac{1}{20}\frac{S_2}{\sqrt{S_1S_3}}\Big(\frac{2}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\mathcal{K}_4^2\Big)\frac{S_4}{S_2} \\ & +840\Big(\mathcal{K}_6^0\mp\frac{1}{35}\frac{S_2}{\sqrt{S_1S_3}}\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\mathcal{K}_6^2\Big)\frac{S_6}{S_2}\Big\} \end{aligned} \tag{5.115}$$

and for $f_b^{\pm}$

$$
\begin{aligned}
f_6(B_l^m, \mathcal{K}_l^m, S_2)^{\pm} = 4S_1 \Big\{ & \frac{9}{2} B_2^0 \Big(\frac{S_2}{\sqrt{S_1 S_3}} \Big(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp \frac{2}{3} \Big) \\
& - 45 B_4^0 \Big(\frac{S_2}{\sqrt{S_1 S_3}} \Big(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp 3 \mp \frac{7}{3} \frac{S_2}{\sqrt{S_4}} \Big) \frac{S_4}{S_2} \\
& + \frac{315}{2} B_6^0 \Big(\frac{S_2}{\sqrt{S_1 S_3}} \Big(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp \frac{20}{3} \mp 6 \frac{S_2}{\sqrt{S_4}} \Big) \frac{S_6}{S_2} \\
& + \frac{45}{2} B_6^6 \cos 6\alpha \Big(\frac{S_2}{\sqrt{S_1 S_3}} \Big(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \pm \frac{28}{3} \pm 2 \frac{S_2}{\sqrt{S_4}} \Big) \frac{S_6}{S_2} \\
& - 3 \Big(\mathcal{K}_2^2 \frac{S_2}{\sqrt{S_1 S_3}} \Big(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp 2 \mathcal{K}_2^0 \Big) \\
& - 18 \Big(\mathcal{K}_4^2 \frac{S_2}{\sqrt{S_1 S_3}} \Big(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp 20 \mathcal{K}_4^0 \mp \frac{4}{3} \frac{S_2}{\sqrt{S_4}} \mathcal{K}_4^4 \Big) \\
& - 48 \Big(\mathcal{K}_6^2 \frac{S_2}{\sqrt{S_1 S_3}} \Big(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \Big) \mp 70 \mathcal{K}_6^0 \mp 5 \frac{S_2}{\sqrt{S_4}} \mathcal{K}_6^6 \Big)
\end{aligned}
$$

(5.116)

The $\mathcal{K}_l^m$ coefficients are defined in the equations (5.70) - (5.77). We find by means of (5.113), (5.114), (5.115) and (5.116) the temperature dependent energy gap

$$
\begin{aligned}
\Delta(T)^2 = \; & \mathcal{A}_0(0) \big[\mathcal{A}_0(0) + (f_M^+ + f_M^-) \Delta M(T) \big] \\
& - \mathcal{B}_0(0) \big[\mathcal{B}_0(0) - (f_M^- - f_M^+) \Delta M(T) \big] \\
& + \big[\mathcal{A}_0(0)(f_6^+ + f_6^-) + \mathcal{B}_0(0)(f_6^- - f_6^+) \big] b(T) \\
& + f_M^+ f_M^- \Delta M(T)^2 + f_6^+ f_6^- b(T)^2 \\
& + (f_M^+ f_6^- + f_M^- f_6^+) \Delta M(T)\, b(T)
\end{aligned}
\qquad (5.117)
$$

Below we set up the energy gap of the heavy rare earths which means for low temperatures the energy gap of a ferromagnetic structure with the moments lying in the hexagonal planes. We find in the infinite spin limit

$$
\begin{aligned}
\Delta(T)^2 = \frac{1}{4}\Big\{ & 36\left(\frac{S_2}{S_1}\right)^2 (B_2^0)^2 \left[m(T)^4 - m(T)^3\right] \\
& + 3600\left(\frac{S_4}{S_1}\right)^2 (B_4^0)^2 \left[m(T)^{18} - m(T)^{17}\right] \\
& + 44100\left(\frac{S_6}{S_1}\right)^2 (B_6^0)^2 \left[m(T)^{40} - m(T)^{39}\right] \\
& + 1764\left(\frac{S_6}{S_1}\right)^2 (B_6^6)^2 \cos^2 6\alpha \left[m(T)^{40} - \frac{25}{49} m(T)^{39}\right] \\
& + 36\left(\frac{S_2}{S_1}\right)^2 (B_{22}^{\gamma})^2 \left[m(T)^4 - \frac{1}{9} m(T)^3\right] \cos^2 2\alpha \\
& + 400\left(\frac{S_4}{S_1}\right)^2 (B_{42}^{\gamma})^2 \left[m(T)^{18} - \frac{9}{25} m(T)^{17}\right] \cos^2 2\alpha \\
& + 400\left(\frac{S_4}{S_1}\right)^2 (B_{44}^{\gamma})^2 \left[m(T)^{18} - \frac{1}{25} m(T)^{17}\right] \cos^2 4\alpha \\
& + 1764\left(\frac{S_6}{S_1}\right)^2 (B_{62}^{\gamma})^2 \left[m(T)^{40} - \left(\frac{17}{21}\right)^2 m(T)^{39}\right] \cos^2 2\alpha \\
& + 1764\left(\frac{S_6}{S_1}\right)^2 (B_{64}^{\gamma})^2 \left[m(T)^{40} - \left(\frac{5}{21}\right)^2 m(T)^{39}\right] \cos^2 4\alpha \\
& - 720 \frac{S_2 S_4}{S_1^2} B_2^0 B_4^0 \left[m(T)^{11} - m(T)^{10}\right] \\
& + 2520 \frac{S_2 S_6}{S_1^2} B_2^0 B_6^0 \left[m(T)^{22} - m(T)^{21}\right] \\
& - 504 \frac{S_2 S_6}{S_1^2} B_2^0 B_6^6 \cos 6\alpha \left[m(T)^{22} + \frac{5}{7} m(T)^{21}\right] \\
& - 25200 \frac{S_4 S_6}{S_1^2} B_4^0 B_6^0 \left[m(T)^{29} - m(T)^{28}\right]
\end{aligned}
$$

$$+5040\,\frac{S_4 S_6}{S_1^2}\,\mathbb{B}_4^0\,\mathbb{B}_6^6\cos 6\alpha\left[m(T)^{29}+\frac{5}{7}\,m(T)^{28}\right]$$

$$-11640\left(\frac{S_6}{S_1}\right)^2\mathbb{B}_6^0\,\mathbb{B}_6^6\cos 6\alpha\left[m(T)^{40}+\frac{5}{7}\,m(T)^{39}\right]$$

$$+72\left(\frac{S_2}{S_1}\right)^2\mathbb{B}_2^0\,\mathbb{B}_{22}^{\gamma}\left[m(T)^{4}+\frac{1}{3}\,m(T)^{3}\right]\cos 2\alpha$$

$$-240\,\frac{S_2 S_4}{S_1^2}\,\mathbb{B}_2^0\,\mathbb{B}_{42}^{\gamma}\left[m(T)^{11}-\frac{3}{5}\,m(T)^{10}\right]\cos 2\alpha$$

$$+240\,\frac{S_2 S_4}{S_1^2}\,\mathbb{B}_2^0\,\mathbb{B}_{44}^{\gamma}\left[m(T)^{11}+\frac{3}{5}\,m(T)^{10}\right]\cos 4\alpha$$

$$+504\,\frac{S_2 S_6}{S_1^2}\,\mathbb{B}_2^0\,\mathbb{B}_{62}^{\gamma}\left[m(T)^{22}-\frac{17}{21}\,m(T)^{21}\right]\cos 2\alpha$$

$$-504\,\frac{S_2 S_6}{S_1^2}\,\mathbb{B}_2^0\,\mathbb{B}_{64}^{\gamma}\left[m(T)^{22}-\frac{5}{21}\,m(T)^{21}\right]\cos 4\alpha$$

$$-720\,\frac{S_2 S_4}{S_1^2}\,\mathbb{B}_4^0\,\mathbb{B}_{22}^{\gamma}\left[m(T)^{11}+\frac{1}{3}\,m(T)^{10}\right]\cos 2\alpha$$

$$+2400\left(\frac{S_4}{S_1}\right)^2\mathbb{B}_4^0\,\mathbb{B}_{42}^{\gamma}\left[m(T)^{18}-\frac{3}{5}\,m(T)^{17}\right]\cos 2\alpha$$

$$-2400\left(\frac{S_4}{S_1}\right)^2\mathbb{B}_4^0\,\mathbb{B}_{44}^{\gamma}\left[m(T)^{18}+\frac{3}{5}\,m(T)^{17}\right]\cos 4\alpha$$

$$-5040\,\frac{S_4 S_6}{S_1^2}\,\mathbb{B}_4^0\,\mathbb{B}_{62}^{\gamma}\left[m(T)^{29}-\frac{17}{21}\,m(T)^{28}\right]\cos 2\alpha$$

$$+5040\,\frac{S_4 S_6}{S_1^2}\,\mathbb{B}_4^0\,\mathbb{B}_{64}^{\gamma}\left[m(T)^{29}-\frac{5}{21}\,m(T)^{28}\right]\cos 4\alpha$$

$$+2520\,\frac{S_2 S_6}{S_1^2}\,\mathbb{B}_6^0\,\mathbb{B}_{22}^{\gamma}\left[m(T)^{22}+m(T)^{21}\right]\cos 2\alpha$$

$$-8400\,\frac{S_4 S_6}{S_1^2}\,\mathbb{B}_6^0\,\mathbb{B}_{42}^{\gamma}\left[m(T)^{29}-\frac{3}{5}\,m(T)^{28}\right]\cos 2\alpha$$

$$+8400\,\frac{S_4S_6}{S_1^2}\,B_6^0\,B_{44}^T\left[m(T)^{29}+\frac{3}{5}\,m(T)^{28}\right]\cos 4\alpha$$

$$+17640\left(\frac{S_6}{S_1}\right)^2 B_6^0\,B_{62}^T\left[m(T)^{40}-\frac{17}{21}\,m(T)^{39}\right]\cos 2\alpha$$

$$-17640\left(\frac{S_6}{S_1}\right)^2 B_6^0\,B_{64}^T\left[m(T)^{40}-\frac{5}{21}\,m(T)^{39}\right]\cos 4\alpha$$

$$-504\,\frac{S_2S_6}{S_1^2}\,B_6^6\,B_{22}^T\left[m(T)^{22}-\frac{5}{21}\,m(T)^{21}\right]\cos 2\alpha\cos 6\alpha$$

$$+1680\,\frac{S_4S_6}{S_1^2}\,B_6^6\,B_{42}^T\left[m(T)^{29}+\frac{3}{7}\,m(T)^{28}\right]\cos 2\alpha\cos 6\alpha$$

$$-1680\,\frac{S_4S_6}{S_1^2}\,B_6^6\,B_{44}^T\left[m(T)^{29}-\frac{3}{7}\,m(T)^{28}\right]\cos 4\alpha\cos 6\alpha$$

$$-3528\left(\frac{S_6}{S_1}\right)^2 B_6^6\,B_{62}^T\left[m(T)^{40}-\frac{85}{147}\,m(T)^{39}\right]\cos 2\alpha\cos 6\alpha$$

$$+3528\left(\frac{S_6}{S_1}\right)^2 B_6^6\,B_{64}^T\left[m(T)^{40}+\frac{25}{147}\,m(T)^{39}\right]\cos 4\alpha\cos 6\alpha$$

$$-240\,\frac{S_2S_4}{S_1^2}\,B_{22}^T\,B_{42}^T\left[m(T)^{11}+\frac{1}{5}\,m(T)^{10}\right]\cos^2 2\alpha$$

$$+240\,\frac{S_2S_4}{S_1^2}\,B_{22}^T\,B_{44}^T\left[m(T)^{11}+\frac{1}{5}\,m(T)^{10}\right]\cos 2\alpha\cos 4\alpha$$

$$+504\,\frac{S_2S_6}{S_1^2}\,B_{22}^T\,B_{62}^T\left[m(T)^{22}+\frac{17}{63}\,m(T)^{21}\right]\cos^2 2\alpha$$

$$-504\,\frac{S_2S_6}{S_1^2}\,B_{22}^T\,B_{64}^T\left[m(T)^{22}+\frac{5}{63}\,m(T)^{21}\right]\cos 2\alpha\cos 4\alpha$$

$$-800\left(\frac{S_4}{S_1}\right)^2 B_{42}^T\,B_{44}^T\left[m(T)^{18}+\frac{9}{25}\,m(T)^{17}\right]\cos 2\alpha\cos 4\alpha$$

$$-1680\,\frac{S_4S_6}{S_1^2}\,B_{42}^T\,B_{62}^T\left[m(T)^{29}-\frac{17}{35}\,m(T)^{28}\right]\cos^2 2\alpha$$

$$+1680\frac{S_4S_6}{S_1^2}B_{42}^{\gamma}B_{64}^{\gamma}\left[m(T)^{29}-\frac{1}{7}m(T)^{28}\right]\cos 2\alpha\cos 4\alpha$$

$$+1680\frac{S_4S_6}{S_1^2}B_{44}^{\gamma}B_{62}^{\gamma}\left[m(T)^{29}+\frac{17}{35}m(T)^{28}\right]\cos 2\alpha\cos 4\alpha$$

$$-1680\frac{S_4S_6}{S_1^2}B_{44}^{\gamma}B_{64}^{\gamma}\left[m(T)^{29}+\frac{1}{7}m(T)^{28}\right]\cos^2 4\alpha$$

$$-3528\left(\frac{S_6}{S_1}\right)^2B_{62}^{\gamma}B_{64}^{\gamma}\left[m(T)^{40}-\frac{85}{441}m(T)^{39}\right]\cos 2\alpha\cos 4\alpha\Big\}$$

$$+g\mu_BH\Big\{6\frac{S_2}{S_1}B_2^0\left(1+m(T)^4\right)-60\frac{S_4}{S_1}B_4^0\left(1+m(T)^{18}\right)$$

$$+210\frac{S_6}{S_1}B_6^0\left(1+m(T)^{40}\right)-42\frac{S_6}{S_1}B_6^6\left(1+m(T)^{40}\right)\cos 6\alpha$$

$$+6\frac{S_2}{S_1}B_{22}^{\gamma}\left(1+m(T)^4\right)\cos 2\alpha-20\frac{S_4}{S_1}B_{42}^{\gamma}\left(1+m(T)^{18}\right)\cos 2\alpha$$

$$+20\frac{S_4}{S_1}B_{44}^{\gamma}\left(1+m(T)^{18}\right)\cos 4\alpha+42\frac{S_6}{S_1}B_{62}^{\gamma}\left(1+m(T)^{40}\right)\cos 2\alpha$$

$$-42\frac{S_6}{S_1}B_{64}^{\gamma}\left(1+m(T)^{40}\right)\cos 4\alpha\Big\}+(g\mu_BH)^2$$

$$+\left[A_0(0)\left(f_6^+ + f_6^-\right)+B_0(0)\left(f_6^- - f_6^+\right)\right]b(T)$$

(5.118)

We have only worked out in details the terms linear in $\Delta M(T)$ and have by means of those terms deduced the power law dependences of the energy gap on the relative magnetization. To calculate the coefficient of the term linear in b(T) in the infinite spin limit the following expressings are necessary

$$\mathcal{A}_0(0) = \Big\{ 6\frac{S_2}{S_1}\mathbb{B}_2^0 - 60\frac{S_4}{S_1}\mathbb{B}_4^0 + 210\frac{S_6}{S_1}\mathbb{B}_6^0 - 42\frac{S_6}{S_1}\mathbb{B}_6^6\cos 6\alpha$$
$$+6\frac{S_2}{S_1}\mathbb{B}_{22}^\gamma\cos 2\alpha - 20\frac{S_4}{S_1}\mathbb{B}_{42}^\gamma\cos 2\alpha + 20\frac{S_4}{S_1}\mathbb{B}_{44}^\gamma\cos 4\alpha$$
$$+42\frac{S_6}{S_1}\mathbb{B}_{62}^\gamma\cos 2\alpha - 42\frac{S_6}{S_1}\mathbb{B}_{64}^\gamma\cos 4\alpha + g\mu_B H\Big\}\times\frac{1}{2} \tag{5.119}$$

$$\mathcal{B}_0(0) = \Big\{-6\frac{S_2}{S_1}\mathbb{B}_2^0 + 60\frac{S_4}{S_1}\mathbb{B}_4^0 - 210\frac{S_6}{S_1}\mathbb{B}_6^0 - 30\frac{S_6}{S_1}\mathbb{B}_6^6\cos 6\alpha$$
$$+2\frac{S_2}{S_1}\mathbb{B}_{22}^\gamma\cos 2\alpha + 12\frac{S_4}{S_1}\mathbb{B}_{42}^\gamma\cos 2\alpha + 12\frac{S_4}{S_1}\mathbb{B}_{44}^\gamma\cos 4\alpha$$
$$-34\frac{S_6}{S_1}\mathbb{B}_{62}^\gamma\cos 2\alpha + 10\frac{S_6}{S_1}\mathbb{B}_{64}^\gamma\cos 4\alpha\Big\}\times\frac{1}{2} \tag{5.120}$$

$$f_6^+ + f_6^- = +S_1\Big\{9\mathbb{B}_2^0 - 300\frac{S_4}{S_2}\mathbb{B}_4^0 + 2205\frac{S_6}{S_2}\mathbb{B}_6^0 + 315\frac{S_6}{S_2}\mathbb{B}_6^6\cos 6\alpha$$
$$-3\mathbb{B}_{22}^\gamma\cos 2\alpha - 60\frac{S_4}{S_2}\mathbb{B}_{42}^\gamma\cos 2\alpha - 60\frac{S_4}{S_2}\mathbb{B}_{44}^\gamma\cos 4\alpha$$
$$+357\frac{S_6}{S_2}\mathbb{B}_{62}^\gamma\cos 2\alpha - 105\frac{S_6}{S_2}\mathbb{B}_{64}^\gamma\cos 4\alpha\Big\} \tag{5.121}$$

$$f_6^- - f_6^+ = 4S_1\Big\{6\mathbb{B}_2^0 - 480\frac{S_4}{S_2}\mathbb{B}_4^0 + 3190\frac{S_6}{S_2}\mathbb{B}_6^0 - 510\frac{S_6}{S_2}\mathbb{B}_6^6\cos 6\alpha$$
$$+6\mathbb{B}_{22}^\gamma\cos 2\alpha - 48\frac{S_4}{S_2}\mathbb{B}_{42}^\gamma\cos 2\alpha + 96\frac{S_4}{S_2}\mathbb{B}_{44}^\gamma\cos 4\alpha$$
$$+510\frac{S_6}{S_2}\mathbb{B}_{62}^\gamma\cos 2\alpha - 30\frac{S_6}{S_2}\mathbb{B}_{64}^\gamma\cos 4\alpha\Big\} \tag{5.122}$$

The short hand notation of $\mathcal{B}_2^0$, $\mathcal{B}_4^0$, $\mathcal{B}_6^0$ and $\mathcal{B}_6^6$ is that of (4.22) - (4.25) whereas we besides have introduced

$$\mathcal{B}_{l,m}^{\gamma} = B_{l,m}^{\gamma}\,\bar{\varepsilon}_1^{\gamma} \tag{5.123}$$

To bring the expression of the energy gap on a shorter form we consider the following schemes

l_1	l_2	$L_1 = l_1(l_1+1)/2-1$	$L_2 = l_2(l_2+1)/2-1$	L_1+L_2
2	2	2	2	4
4	4	9	9	18
6	6	20	20	40
2	4	2	9	11
2	6	2	20	22
4	6	9	20	29

l_1	l_2	$L_1 = l_1(l_1+1) - \frac{3}{2}$	$L_2 = l_2(l_2+1) - \frac{3}{2}$	L_1+L_2
2	2	3/2	3/2	3
4	4	17/2	17/2	17
6	6	39/2	39/2	39
2	4	3/2	17/2	10
2	6	3/2	39/2	21
4	6	17/2	39/2	28

From the numbers of the two schemes we deduce the temperature dependence of the energy gap as a power law of the relative magnetization plus the term linear in b(T)

$$\begin{aligned}\Delta(T)^2 = \sum_{l_1 m_1}\sum_{l_2 m_2} &\mathcal{C}_{l_1,m_1}\,\mathcal{C}_{l_2 m_2}\,\frac{S_{l_1}S_{l_2}}{S_1^2}\,\mathcal{B}_{l_1 m_1}\,\mathcal{B}_{l_2 m_2}\,\cdot \\ &\Big[m(T)^{l_1(l_1+1)/2-1}\; m(T)^{l_2(l_2+1)/2-1} \\ &+K(l_1 m_1 l_2 m_2)\,m(T)^{l_1(l_1+1)/2-\frac{3}{2}}\; m(T)^{l_2(l_2+1)/2-3/2}\Big] \\ &+ K(\mathcal{B}_l^m,\ \mathcal{B}_{l,m}^{\gamma},\ S_l)\ b(T)\end{aligned} \tag{5.124}$$

This formula is in a very short hand notation to be able to express the dependences of the energy gap of the relative magnetization.

We finish this section by setting up the energy gap when only the anisotropy parameters B_2^0 and B_6^6 are left. This is the shortest way to give a formula that is still realistic of the heavy rare earths. From (5.118) we find

$$
\begin{aligned}
\Delta(T)^2 = \tfrac{1}{4}\Big\{ & 36\left(\frac{S_2}{S_1}\right)^2 (B_2^0)^2 \left[m(T)^4 - m(T)^{12} \right] \\
& + 1764\left(\frac{S_6}{S_1}\right)^2 (B_6^6)^2 \left[m(T)^{40} - \frac{25}{49} m(T)^{84} \right] \cos^2 6\alpha \\
& - 504\, \frac{S_2 S_6}{S_1^2} B_2^0 B_6^6 \left[m(T)^{22} + \frac{5}{7} m(T)^{48} \right] \cos 6\alpha \Big\} \\
& + 72 \Big\{ S_2 (B_2^0)^2 + 115\left(\frac{S_6}{S_1}\right)^2 (B_6^6)^2 \cos^2 6\alpha \\
& \qquad + 244\, S_6 B_2^0 B_6^6 \cos 6\alpha \Big\}\, \sigma(T)
\end{aligned}
\tag{5.125}
$$

6. THEORY OF FERROMAGNETIC RESONANS

A phenomenological macroscopic theory of ferromagnetic resonance has been developed by Smit and Beljers[30]. The ferromagnetic resonance frequency is the frequency of the $q = 0$ spin wave mode of the magnetized crystal. The magnetic free energy $\mathcal{F}(T, \underline{H})$ for constant T and $\underline{H}$ is a function of the orientation of the magnetization vector, $\mathcal{F}(\theta, \varphi)$. Let the equilibrium direction of the magnetization vector be the ζ-direction, and the small angles of deviation in two perpendicular directions θ and φ. Then the equations of motion of the magnetization vector $\underline{M}$ are

$$
-M\dot{\theta} = \gamma \frac{\partial \mathcal{F}(\theta,\varphi)}{\partial \varphi} \tag{6.1}
$$

$$
M\dot{\varphi} = \gamma \frac{\partial \mathcal{F}(\theta,\varphi)}{\partial \theta} \tag{6.2}
$$

γ is the gyromagnetic ratio, equal to $\gamma = g\mu_B/\hbar$

g is the Lande's splitting factor, μ_β the Bohr magneton and h the Planck constant.

(The equations of motion are in reality nothing else than the classical Hamilton equations of motion for the set of conjugate variables $(\varphi, \frac{M}{\gamma}\theta)$). For small deviations from the equilibrium position we may use for the free energy the first terms of a Taylor Series

$$\mathcal{F}(\theta,\varphi) = \mathcal{F}_0 + \frac{1}{2}\left(\mathcal{F}_{\theta\theta}\,\theta^2 + 2\mathcal{F}_{\theta\varphi}\,\theta\varphi + \mathcal{F}_{\varphi\varphi}\,\varphi^2\right) \qquad (6.3)$$

In the equilibrium position we have $\mathcal{F}_\theta = 0$; $\mathcal{F}_\varphi = 0$. The symbols used mean

$$\mathcal{F}_\theta = \frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\theta}\ ; \qquad \mathcal{F}_\varphi = \frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\varphi} \qquad (6.4)$$

$$\mathcal{F}_{\theta\theta} = \frac{\partial^2 \mathcal{F}(\theta,\varphi)}{\partial\theta^2}\ ; \quad \mathcal{F}_{\theta\varphi} = \frac{\partial^2 \mathcal{F}(\theta,\varphi)}{\partial\theta\,\partial\varphi}\ ; \quad \mathcal{F}_{\varphi\varphi} = \frac{\partial^2 \mathcal{F}(\theta,\varphi)}{\partial\varphi^2} \qquad (6.5)$$

$$\frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\varphi} = \mathcal{F}_{\theta\varphi}\,\theta + \mathcal{F}_{\varphi\varphi}\,\varphi \qquad (6.6)$$

$$\frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\theta} = \mathcal{F}_{\theta\theta}\,\theta + \mathcal{F}_{\theta\varphi}\,\varphi \qquad (6.7)$$

for which reason

$$-M\dot{\theta} = \gamma\left(\mathcal{F}_{\theta\varphi}\,\theta + \mathcal{F}_{\varphi\varphi}\,\varphi\right) \qquad (6.8)$$

$$M\dot{\varphi} = \gamma\left(\mathcal{F}_{\theta\theta}\,\theta + \mathcal{F}_{\theta\varphi}\,\varphi\right) \qquad (6.9)$$

Suppose the solutions of these equations vary harmonically in time with the angular frequency ω , that is

$$\begin{aligned} \theta &= \theta_0 \, e^{i\omega t} \\ \varphi &= \varphi_0 \, e^{i\omega t} \end{aligned} \qquad (6.10)$$

then

$$\begin{bmatrix} \gamma \mathcal{F}_{\theta\varphi} + i\omega M & \gamma \mathcal{F}_{\varphi\varphi} \\ \gamma \mathcal{F}_{\theta\theta} & \gamma \mathcal{F}_{\theta\varphi} - i\omega M \end{bmatrix} \begin{bmatrix} \theta \\ \varphi \end{bmatrix} = 0$$

from where we immediately find the frequency

$$\hbar\omega = \frac{g\mu_0}{M} \sqrt{\mathcal{F}_{\theta\theta}\mathcal{F}_{\varphi\varphi} - (\mathcal{F}_{\theta\varphi})^2} \qquad (6.11)$$

From statistical mechanics we have for the free energy

$$\mathcal{F}(\theta,\varphi) = -k_B T \ln Tr \left\{ e^{-\mathcal{H}(\theta,\varphi)/k_B T} \right\} \qquad (6.12)$$

$\mathcal{H}(\theta,\varphi)$ is the Hamiltonian of the system and (θ,φ) the direction of the magnetization with respect to crystal axes. We find after differentiating the free energy:

$$\mathcal{F}_\theta = \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \theta} \right\rangle ; \quad \mathcal{F}_\varphi = \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \varphi} \right\rangle \qquad (6.13)$$

$$\hat{f}_{\theta\theta} = \left\langle \frac{\partial^2 \mathcal{H}(\theta,\varphi)}{\partial \theta^2} \right\rangle + \frac{1}{k_B T} \left[\left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \theta} \right\rangle^2 - \left\langle \left(\frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \theta} \right)^2 \right\rangle \right] \qquad (6.14)$$

$$\mathcal{F}_{\varphi\varphi} = \left\langle \frac{\partial^2 \mathcal{H}(\theta,\varphi)}{\partial \varphi^2} \right\rangle + \frac{1}{k_B T}\left[\left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \varphi} \right\rangle^2 - \left\langle \left(\frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \varphi} \right)^2 \right\rangle \right] \tag{6.15}$$

$$\mathcal{F}_{\theta,\varphi} = \left\langle \frac{\partial^2 \mathcal{H}(\theta,\varphi)}{\partial \theta \partial \varphi} \right\rangle + \frac{1}{k_B T}\left[\left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \theta} \right\rangle \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \varphi} \right\rangle - \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \theta} \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial \varphi} \right\rangle \right] \tag{6.16}$$

Using these formulae for a system with a specified Hamiltonian $\mathcal{H}(\theta,\varphi)$. (6.11) gives the q = 0 frequency.

Without taking into account magnetostriction we consider the single ion anisotropy of a hexagonal lattice, given by (5.7) and calculate on this basis the temperature dependent resonans frequency. In the c-representation the anisotropy is given by

$$\mathcal{H}_{an} = \sum_{l} \left\{ B_2^0 O_2^0(c) + B_4^0 O_4^0(c) + B_6^0 O_6^0(c) + B_6^6 O_6^6(c) \right\}_l \tag{6.17}$$

However, we want to treat the case with the magnetization lying in the basal plane for which reason a rotation of the anisotropy must be performed. By means of table 6 of Rotated Stevens Operators we set up a rotation of the anisotropy through the angles θ and φ. We find

$$\begin{aligned}
\mathcal{H}_{an}(\theta,\varphi) = \sum_{l} \Big\{ & B_2^0 \Big[\tfrac{1}{2}(3\cos^2\theta - 1)\, O_2^0(c) - \tfrac{3}{2}\sin^2\theta\, O_2^2(c) \\
& \quad + 3\sin\theta\cos\theta\, O_2^1(s) \Big] + \\
& B_4^0 \Big[\tfrac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3)\, O_4^0(c) + \tfrac{35}{8}\sin^4\theta\, O_4^4(c) \\
& \quad - \tfrac{5}{2}\sin^2\theta\,(7\cos^2\theta - 1)\, O_4^2(c) - 35\cos\theta\sin^3\theta\, O_4^3(s) \\
& \quad + 5\sin\theta\cos\theta\,(7\cos^2\theta - 3)\, O_4^1(s) \Big] + \\
& B_6^0 \Big[\tfrac{1}{16}(231\cos^6\theta - 315\cos^4\theta + 105\cos^2\theta - 5)\, O_6^0(c)
\end{aligned}$$

$$- \frac{231}{32} \sin^6\theta \, O_6^6(c) + \frac{63}{16}(11\cos^2\theta - 1)\sin^4\theta \, O_6^4(c)$$

$$- \frac{105}{32}(33\cos^4\theta - 18\cos^2\theta + 1)\sin^2\theta \, O_6^2(c)$$

$$+ \frac{231}{8}\cos\theta \sin^5\theta \, O_6^5(s) - \frac{105}{8}(11\cos^3\theta - 3\cos\theta)\sin^3\theta \, O_6^3(s)$$

$$+ \frac{21}{4}(33\cos^5\theta - 30\cos^3\theta + 5\cos\theta)\sin\theta \, O_6^1(s) \Big]$$

$$+ B_6^6 \Big[\frac{1}{16}\sin^6\theta \, O_6^0(c) - \frac{1}{32}(1 + 15\cos^2\theta + 15\cos^4\theta + \cos^6\theta) O_6^6(c)$$

$$+ \frac{3}{16}\sin^2\theta(1 + 6\cos^2\theta + \cos^4\theta) O_6^4(c)$$

$$- \frac{15}{32}\sin^4\theta(1 + \cos^2\theta) O_6^2(c)$$

$$+ \frac{5}{2}\sin^3\theta(\cos^3\theta + 3\cos\theta) O_6^3(s)$$

$$- \frac{3}{4}\sin^5\theta \cos\theta \, O_6^1(s)$$

$$- \frac{3}{8}\sin\theta(\cos^5\theta + 10\cos^3\theta + 5\cos\theta) O_6^5(s) \Big] \cos 6\varphi$$

$$+ B_6^6 \Big[\frac{1}{32}(3\cos\theta + 10\cos^3\theta + 3\cos^5\theta) O_6^6(s)$$

$$- \frac{3}{4}\sin^4\theta(\cos\theta + \cos^3\theta) O_6^4(s)$$

$$+ \frac{15}{16}\sin^4\theta \cos\theta \, O_6^2(s) - \frac{3}{8}\sin\theta(1 + 10\cos^2\theta + 5\cos^4\theta) O_6^5(s)$$

$$+ \frac{5}{2}\sin^3\theta(1 + 3\cos^2\theta) O_6^3(c) - \frac{3}{4}\sin^5\theta \, O_6^1(c) \Big] \sin 6\varphi \Big\}$$

(6.18)

On the basis of this cumbersome expression the quantities (6.14) - (6.16), to be put into the frequency formula (6.11), have been calculated for $\theta = \frac{\pi}{2}$, which gives

$$
\begin{aligned}
\mathcal{F}_{\theta\theta} = \sum_{l} \Big\{ & 3B_2^0\left(\langle O_2^0(c)\rangle + \langle O_2^2(c)\rangle\right) \\
& - \frac{15}{2} B_4^0\left(\langle O_4^0(c)\rangle + 8\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\right) \\
& + \frac{21}{16} B_6^0\left(10\langle O_6^0(c)\rangle + 95\langle O_6^2(c)\rangle + 78\langle O_6^4(c)\rangle + 33\langle O_6^6(c)\rangle\right) \\
& - \frac{3}{15} B_6^6\left(2\langle O_6^0(c)\rangle + 5\langle O_6^2(c)\rangle + \langle O_6^4(c)\rangle - 5\langle O_6^6(c)\rangle\right)\cos 6\varphi \Big\} \\
- \frac{1}{k_B T}\sum_{l} \Big\{ & 9B_2^0\langle O_2^1(s)\, O_2^1(s)\rangle + B_4^0\Big[75\langle O_4^1(s)\, O_4^1(s)\rangle \\
& + 1225\langle O_4^3(s)\, O_4^3(s)\rangle + 525\left(\langle O_4^3(s)\, O_4^1(s)\rangle\right. \\
& \left. + \langle O_4^1(s)\, O_4^3(s)\rangle\right)\Big] + B_6^0\Big[\left(\frac{105}{4}\right)^2\langle O_6^1(s)\, O_6^1(s)\rangle \\
& + \left(\frac{315}{8}\right)^2\langle O_6^3(s)\, O_6^3(s)\rangle + \left(\frac{231}{8}\right)^2\langle O_6^5(s)\, O_6^5(s)\rangle \\
& + \frac{3}{2}\left(\frac{105}{4}\right)^2\left(\langle O_6^1(s)\, O_6^3(s)\rangle + \langle O_6^3(s)\, O_6^1(s)\rangle\right) \\
& + \frac{105}{4}\,\frac{231}{8}\left(\langle O_6^1(s)\, O_6^5(s)\rangle + \langle O_6^5(s)\, O_6^1(s)\rangle\right) \\
& + \frac{315}{8}\cdot\frac{231}{8}\left(\langle O_6^3(s)\, O_6^5(s)\rangle + \langle O_6^5(s)\, O_6^3(s)\rangle\right)\Big]\Big\} \\
- \frac{1}{k_B T}\sum_{l} B_6^6 \Big\{ & \frac{225}{64}\Big[\langle O_6^3(s)\, O_6^3(s)\rangle + \langle O_6^5(s)\, O_6^5(s)\rangle \\
& - \left(\langle O_6^3(s)\, O_6^5(s)\rangle + \langle O_6^5(s)\, O_6^3(s)\rangle\right)\Big]\cos^2 6\varphi
\end{aligned}
$$

$$
\begin{aligned}
&+\Big[\tfrac{225}{256}\langle O_6^2(s)\,O_6^2(s)\rangle+\tfrac{9}{16}\langle O_6^4(s)\,O_6^4(s)\rangle \\
&\quad+\tfrac{9}{1024}\langle O_6^6(s)\,O_6^6(s)\rangle-\tfrac{45}{64}\big(\langle O_6^2(s)\,O_6^4(s)\rangle \\
&\quad+\langle O_6^4(s)\,O_6^2(s)\rangle\big) \\
&\quad+\tfrac{45}{512}\big(\langle O_6^2(s)\,O_6^6(s)\rangle+\langle O_6^6(s)\,O_6^2(s)\rangle\big) \\
&\quad-\tfrac{9}{128}\big(\langle O_6^4(s)\,O_6^6(s)\rangle+\langle O_6^6(s)\,O_6^4(s)\rangle\big)\Big]\sin^2 6\varphi \\
&+\Big[\tfrac{225}{128}\big(\langle O_6^3(s)\,O_6^2(s)\rangle+\langle O_6^2(s)\,O_6^3(s)\rangle\big) \\
&\quad-\tfrac{45}{32}\big(\langle O_6^3(s)\,O_6^4(s)\rangle+\langle O_6^4(s)\,O_6^3(s)\rangle\big) \\
&\quad+\tfrac{45}{256}\big(\langle O_6^3(s)\,O_6^6(s)\rangle+\langle O_6^6(s)\,O_6^3(s)\rangle\big) \\
&\quad-\tfrac{225}{128}\big(\langle O_6^5(s)\,O_6^2(s)\rangle+\langle O_6^2(s)\,O_6^5(s)\rangle\big) \\
&\quad+\tfrac{45}{32}\big(\langle O_6^5(s)\,O_6^4(s)\rangle+\langle O_6^4(s)\,O_6^5(s)\rangle\big) \\
&\quad-\tfrac{45}{128}\big(\langle O_6^5(s)\,O_6^6(s)\rangle+\langle O_6^6(s)\,O_6^5(s)\rangle\big)\Big]\cdot \\
&\qquad\cdot\cos 6\varphi\,\sin 6\varphi\Big\}_l
\end{aligned}
\tag{6.19}
$$

$$
\begin{aligned}
\mathcal{F}_{\varphi\varphi} = \sum_{\ell} \Big\{ & -\tfrac{9}{8} B_6^6 \left[2\langle O_6^0(c)\rangle - 15\langle O_6^2(c)\rangle + 6\langle O_6^4(c)\rangle - \langle O_6^6(c)\rangle \right] \cos 6\varphi \Big\}_{\ell} \\
& - \frac{1}{k_B T} \sum_{\ell} \Big\{ \frac{9}{16} \langle O_6^1(c) O_6^1(c)\rangle + \frac{25}{64} \langle O_6^3(c) O_6^3(c)\rangle + \frac{9}{64} \langle O_6^5(c) O_6^5(c)\rangle \\
& \qquad - \frac{15}{32} \left(\langle O_6^3(c)\, O_6^1(c)\rangle + \langle O_6^1(c)\, O_6^3(c)\rangle \right) \\
& \qquad - \frac{15}{64} \left(\langle O_6^3(c)\, O_6^5(c)\rangle + \langle O_6^5(c)\, O_6^3(c)\rangle \right) \\
& \qquad + \frac{9}{32} \left(\langle O_6^1(c)\, O_6^5(c)\rangle + \langle O_6^5(c)\, O_6^1(c)\rangle \right) \Big\}_{\ell} \times \\
& \qquad \times 36\, B_6^6 \cos^2 6\varphi
\end{aligned}
\tag{6.20}
$$

$$
\begin{aligned}
\mathcal{F}_{\theta\varphi} = \frac{1}{k_B T} \sum_{\ell} B_6^6 \Big\{ & \Big[\frac{45}{32} \langle O_6^1(c)\, O_6^3(s)\rangle - \frac{75}{64} \langle O_6^3(c)\, O_6^3(s)\rangle \\
& + \frac{45}{64} \langle O_6^5(c)\, O_6^3(s)\rangle - \frac{45}{32} \langle O_6^1(c)\, O_6^5(s)\rangle \\
& + \frac{75}{64} \langle O_6^3(c)\, O_6^5(s)\rangle - \frac{45}{64} \langle O_6^5(c)\, O_6^5(s)\rangle \Big] \times \\
& \times 6 \cos^2 6\varphi \\
& - \Big[\frac{1}{16} \langle O_6^0(c)\, O_6^3(s)\rangle + \frac{225}{256} \langle O_6^2(c)\, O_6^3(s)\rangle \\
& - \frac{45}{128} \langle O_6^4(c)\, O_6^3(s)\rangle + \frac{15}{128} \langle O_6^6(c)\, O_6^3(s)\rangle \\
& + \frac{1}{16} \langle O_6^0(c)\, O_6^5(s)\rangle - \frac{225}{128} \langle O_6^2(c)\, O_6^5(s)\rangle
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{45}{128}\langle O_6^4(c)\,O_6^5(s)\rangle-\frac{15}{128}\langle O_6^6(c)\,O_6^5(s)\rangle\\
&-\frac{45}{64}\langle O_6^1(c)\,O_6^2(s)\rangle+\frac{9}{16}\langle O_6^1(c)\,O_6^4(s)\rangle\\
&-\frac{9}{128}\langle O_6^1(c)\,O_6^6(s)\rangle+\frac{75}{128}\langle O_6^3(c)\,O_6^2(c)\rangle\\
&-\frac{15}{32}\langle O_6^3(c)\,O_6^4(s)\rangle+\frac{15}{256}\langle O_6^6(s)\,O_6^3(c)\rangle\\
&-\frac{45}{128}\langle O_6^5(c)\,O_6^2(s)\rangle+\frac{9}{32}\langle O_6^5(c)\,O_6^4(s)\rangle\\
&-\frac{9}{256}\langle O_6^5(c)\,O_6^6(s)\rangle\Big]\cdot 6\sin 6\varphi\cos 6\varphi\\
-\Big[&-\frac{15}{256}\langle O_6^0(c)\,O_6^2(s)\rangle+\frac{3}{48}\langle O_6^0(c)\,O_6^4(s)\rangle\\
&-\frac{3}{512}\langle O_6^0(c)\,O_6^6(s)\rangle+\frac{225}{512}\langle O_6^2(c)\,O_6^2(s)\rangle\\
&-\frac{45}{64}\langle O_6^2(c)\,O_6^4(s)\rangle+\frac{45}{1024}\langle O_6^2(c)\,O_6^6(s)\rangle\\
&-\frac{45}{256}\langle O_6^4(c)\,O_6^2(s)\rangle+\frac{9}{64}\langle O_6^4(c)\,O_6^4(s)\rangle\\
&-\frac{9}{512}\langle O_6^4(c)\,O_6^6(s)\rangle+\frac{15}{512}\langle O_6^6(c)\,O_6^2(s)\rangle\\
&-\frac{3}{128}\langle O_6^6(c)\,O_6^4(s)\rangle+\frac{3}{1024}\langle O_6^6(c)\,O_6^6(s)\rangle\Big]\cdot\\
&\qquad 6\sin^2 6\varphi\Big\}_l
\end{aligned}
$$

(6.21)

These second derivatives of the free energy are put into the frequency formula with the two cases, $\varphi = 0$ and $\varphi = 30^{\circ}$. Omitting the summation signs we find, keeping the correlation functions on closed form in the frequency expression.

$$\hbar\omega(0) = \frac{g\mu_B}{M(T)}\Bigg\{ \mp\frac{9}{8}\Big(2\langle O_6^0(c)\rangle - 15\langle O_6^2(c)\rangle + 6\langle O_6^4(c)\rangle\Big) \times$$

$$\cdot\Big[3B_2^0B_6^6\big(\langle O_2^0(c)\rangle + \langle O_2^2(c)\rangle\big) - \frac{15}{2}B_4^0B_6^6\big(\langle O_4^0(c)\rangle$$

$$+ 8\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\big) + \frac{21}{16}B_6^0B_6^6\big(10\langle O_6^0(c)\rangle$$

$$+ 95\langle O_6^2(c)\rangle + 78\langle O_6^4(c)\rangle\big) \mp \frac{3}{16}(B_6^6)^2\big(2\langle O_6^0(c)\rangle$$

$$+ 5\langle O_6^2(c)\rangle + \langle O_6^4(c)\rangle\big)\Big]$$

$$-\frac{1}{k_BT}\Bigg[\Bigg[36\Big[\frac{9}{16}\langle O_6^1(c)\,O_6^1(c)\rangle + \frac{25}{64}\langle O_6^3(c)\,O_6^3(c)\rangle$$

$$+\frac{9}{64}\langle O_6^5(c)\,O_6^5(c)\rangle$$

$$-\frac{15}{32}\big(\langle O_6^3(c)\,O_6^1(c)\rangle + \langle O_6^1(c)\,O_6^3(c)\rangle\big)$$

$$+\frac{9}{32}\big(\langle O_6^5(c)\,O_6^1(c)\rangle + \langle O_6^1(c)\,O_6^5(c)\rangle\big)$$

$$-\frac{15}{64}\big(\langle O_6^3(c)\,O_6^5(c)\rangle + \langle O_6^5(c)\,O_6^3(c)\rangle\big)\Big] \times$$

$$\cdot\Big[3B_2^0B_6^6\big(\langle O_2^0(c)\rangle + \langle O_2^2(c)\rangle\big)$$

$$-\frac{15}{2}B_4^0B_6^6\big(\langle O_4^0(c)\rangle + 8\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\big)$$

$$+\frac{21}{16} B_6^0 B_6^6 \left(10\langle O_6^0(c)\rangle + 95\langle O_6^2(c)\rangle + 78\langle O_6^4(c)\rangle\right)$$

$$\mp \frac{3}{16}(B_6^6)^2 \left(2\langle O_6^0(c)\rangle + 5\langle O_6^2(c)\rangle + \langle O_6^4(c)\rangle\right)\Big]$$

$$\mp \frac{9}{8}\left[2\langle O_6^0(c)\rangle - 15\langle O_6^2(c)\rangle + 6\langle O_6^4(c)\rangle\right] \times$$

$$\times\Big[9 B_2^0 B_6^6 \langle O_2^1(s) O_2^1(s)\rangle + 75 B_4^0 B_6^6 \langle O_4^1(s) O_4^1(s)\rangle$$

$$+1225 B_4^0 B_6^6 \langle O_4^3(s) O_4^3(s)\rangle + \left(\frac{105}{4}\right)^2 B_6^0 B_6^6 \langle O_6^1(s) O_6^1(s)\rangle$$

$$+\left(\frac{315}{8}\right)^2 B_6^0 B_6^6 \langle O_6^3(s) O_6^3(s)\rangle + \left(\frac{231}{8}\right)^2 B_6^0 B_6^6 \langle O_6^5(s) O_6^5(s)\rangle$$

$$+525 B_4^0 B_6^6 \left(\langle O_4^3(s) O_4^1(s)\rangle + \langle O_4^1(s) O_4^3(s)\rangle\right)$$

$$+\frac{3}{2}\left(\frac{105}{4}\right)^2 B_6^0 B_6^6 \left(\langle O_6^1(s) O_6^3(s)\rangle + \langle O_6^3(s) O_6^1(s)\rangle\right)$$

$$+\frac{105\cdot 231}{32} B_6^0 B_6^6 \left(\langle O_6^1(s) O_6^5(s) + \langle O_6^5(s) O_6^1(s)\rangle\right)$$

$$+\frac{315\cdot 231}{64} B_6^0 B_6^6 \left(\langle O_6^3(s) O_6^5(s)\rangle + \langle O_6^5(s) O_6^3(s)\rangle\right)$$

$$+\frac{225}{64}(B_6^6)^2 \langle O_6^3(s) O_6^3(s)\rangle + \frac{225}{64}(B_6^6)^2 \langle O_6^5(s) O_6^5(s)\rangle$$

$$-\frac{225}{64}(B_6^6)^2 \left(\langle O_6^3(s) O_6^5(s)\rangle + \langle O_6^5(s) O_6^3(s)\rangle\right)\Big]\Big]$$

$$
\begin{aligned}
+\left(\frac{1}{k_B T}\right)^2 \Bigg[\!\!\Bigg[36 \Big[& \frac{9}{16} \langle O_6^1(c)\, O_6^1(c) \rangle + \frac{25}{64} \langle O_6^3(c)\, O_6^3(c) \rangle \\
& + \frac{9}{64} \langle O_6^5(c)\, O_6^5(c) \rangle \\
& - \frac{15}{32} \left(\langle O_6^3(c)\, O_6^1(c) \rangle + \langle O_6^1(c)\, O_6^3(c) \rangle \right) \\
& + \frac{9}{32} \left(\langle O_6^5(c)\, O_6^1(c) \rangle + \langle O_6^1(c)\, O_6^5(c) \rangle \right) \\
& - \frac{15}{64} \left(\langle O_6^3(c)\, O_6^5(c) \rangle + \langle O_6^5(c)\, O_6^3(c) \rangle \right) \Big] \times \\
& \times \Big[9 B_2^0 B_6^6 \langle O_2^1(s)\, O_2^1(s) \rangle + 75 B_4^0 B_6^6 \langle O_4^1(s)\, O_4^1(s) \rangle \\
& + 1225 B_4^0 B_6^6 \langle O_4^3(s)\, O_4^3(s) \rangle + \left(\frac{105}{4}\right)^2 B_6^0 B_6^6 \langle O_6^1(s)\, O_6^1(s) \rangle \\
& + \left(\frac{315}{8}\right)^2 B_6^0 B_6^6 \langle O_6^3(s)\, O_6^3(s) \rangle + \left(\frac{231}{8}\right)^2 B_6^0 B_6^6 \langle O_6^5(s)\, O_6^5(s) \rangle \\
& + 525 B_4^0 B_6^6 \left(\langle O_4^3(s)\, O_4^1(s) \rangle + \langle O_4^1(s)\, O_4^3(s) \rangle \right) \\
& + \frac{3}{2} \left(\frac{105}{4}\right)^2 B_6^0 B_6^6 \left(\langle O_6^1(s)\, O_6^3(s) \rangle + \langle O_6^3(s)\, O_6^1(s) \rangle \right) \\
& + \frac{105 \cdot 231}{32} B_6^0 B_6^6 \left(\langle O_6^1(s)\, O_6^5(s) \rangle + \langle O_6^5(s)\, O_6^1(s) \rangle \right) \\
& + \frac{315 \cdot 231}{64} B_6^0 B_6^6 \left(\langle O_6^3(s)\, O_6^5(s) \rangle + \langle O_6^5(s)\, O_6^3(s) \rangle \right) \\
& + \frac{225}{64} (B_6^6)^2 \left(\langle O_6^3(s)\, O_6^3(s) \rangle + \langle O_6^5(s)\, O_6^5(s) \rangle \right) \\
& - \frac{225}{64} (B_6^6)^2 \left(\langle O_6^3(s)\, O_6^5(s) \rangle + \langle O_6^5(s)\, O_6^3(s) \rangle \right) \Big] \Bigg]\!\!\Bigg]
\end{aligned}
$$

$$- \left(\tfrac{45}{32}\right)^2 (A_6^6)^2 \Big[\, 6\langle O_6^1(c)\, O_6^3(s)\rangle - 6\langle O_6^1(c)\, O_6^5(s)\rangle - 5\langle O_6^3(c)\, O_6^3(s)\rangle + 5\langle O_6^3(c)\, O_6^5(s)\rangle + 3\langle O_6^5(c)\, O_6^3(s)\rangle - 3\langle O_6^5(c)\, O_6^5(s)\rangle\Big]^2 \Big]\Big]\Big\}^{1/2} \qquad (6.22)$$

The correlation functions of the Racah Operators are calculated by means of the expression of the product of two non-commuting Racah Operators given in (A2.8), namely the following

$$\tilde{O}_{K_1,q_1}(i)\, \tilde{O}_{K_2,q_2}(i) = \sum_{K_3 q_3} (-1)^{K_1+K_2+K_3} (2K_3+1) \begin{pmatrix} K_1 & K_2 & K_3 \\ q_1 & q_2 & q_3 \end{pmatrix} \times \begin{Bmatrix} K_1 & K_2 & K_3 \\ J & J & J \end{Bmatrix} \frac{\langle J \| \tilde{O}_{K_1}(i) \| J\rangle \langle J \| \tilde{O}_{K_2}(i) \| J\rangle}{\langle J \| \tilde{O}_{K_3}(i) \| J\rangle} \tilde{O}^{\dagger}_{K_3 q_3}(i) \qquad (6.23)$$

All the necessary correlation functions are gathered in table 10 to which we refer for numerical calculations.

7. TEMPERATURE DEPENDENCE OF MACROSCOPIC ANISOTROPY CONSTANTS OF HEXAGONAL FERROMAGNETIC CRYSTALS

When the magnetization of a ferromagnetic single crystal is measured as a function of an external, applied magnetic field it is found that in some special directions - the easy directions - much smaller magnetic fields are needed to magnetize the crystal than in other directions. So the energy of the crystal depends on the direction of the magnetization relative to the crystal-axes. The free energy of the crystal accordingly contains a component, which depends on the direction of the spontaneaus magnetization and which is minimum when the magnetization is parallel or antiparallel to the easy direction.

This part of the free energy is the macroscopic magneto crystalline anisotropy. When it is expanded after the direction cosines α_i of the magnetization Birss[31] has shown that for a ferromagnetic hexagonal crystal to the 6th order in α_i the magneto crystalline anisotropy might be written

$$\mathcal{F}(\alpha_1,\alpha_2,\alpha_3) = K_0(T) + K_1(T)\,(\alpha_1^2+\alpha_2^2) + K_2(T)\,(\alpha_1^2+\alpha_2^2)^2 + K_3(T)(\alpha_1^2+\alpha_2^2)^3 + K_4(T)\,(\alpha_1^2-\alpha_2^2)(\alpha_1^4-14\alpha_1^2\alpha_2^2+\alpha_2^4) + \cdots \tag{7.1}$$

$K_0(T)$, $K_1(T)$, $K_2(T)$, $K_3(T)$ and $K_4(T)$ are the temperature dependent anisotropy constants.

The direction cosines are expressible in spherical coordinates (θ,φ) allowing a transformation of the free energy from dependence on the direction cosines to a dependence on spherical coordinates. In appendix (9) it is shown that this transformation gives the following expression of the free energy

$$\mathcal{F}(\theta,\varphi) = K_0(T) + K_1(T)\sin^2\theta + K_2(T)\sin^4\theta + K_3(T)\sin^6\theta + K_4(T)\sin^6\theta\cos 6\varphi + \cdots \tag{7.2}$$

In the section of magnetic resonance we established different connections between the free energy of a magnetic crystal and the Hamiltonian of the crystal. Through these relations we connect the macroscopic anisotropy constants with the microscopic Hamiltonian of the magnetic crystal opening the possibility to calculate the macroscopic constants from microscopic quantities. From (6.13) we find

$$\frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\theta} = \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial\theta} \right\rangle \tag{7.3}$$

$$\frac{\partial \mathcal{F}(\theta,\varphi)}{\partial\varphi} = \left\langle \frac{\partial \mathcal{H}(\theta,\varphi)}{\partial\varphi} \right\rangle \tag{7.4}$$

From (7.2) we immediately find.

$$\frac{\partial F(\theta,\varphi)}{\partial\theta} = K_1(T)\sin 2\theta + 2K_2(T)\sin^2\theta \sin 2\theta$$

$$+3K_3(T)\sin^4\theta \sin 2\theta + 3K_4(T)\sin^4\theta \sin 2\theta \cos 6\varphi \tag{7.5}$$

$$\frac{\partial F(\theta,\varphi)}{\partial\varphi} = -6\,K_4(T)\sin^6\theta \sin 6\varphi \tag{7.6}$$

We want to calculate the macroscopic anisotropy constants for some heavy rare earth metals. They have a hcp-lattice, built up from two interpenetrating hexagonal sublattices. In section (5) on spin waves in the heavy rare earths we took the Hamiltonian to consists of isotrop exchange, single-ion anisotropy and single ion magnetostriction besides a term coming from an externally applied magnetic field. The isotrop exchange is independent of the direction of magnetization, whereas the single ion anisotropy and the single ion magnetostriction are direction dependent. The easy directions of the heavy rare earths are in the basal plane, which requires a rotation of the Stevens operators in the anisotropy - and magnetostriction parts of the Hamiltonlan. Such rotations of Stevens operators and the necessary differentiations are performed in table 6 and table 7.

Taking into account the anisotropy part of the Hamiltonian alone we find

$$K_1(T) = \sum_{l}\Big\{-\tfrac{3}{2}B_2^0\left(\langle O_2^0(l)\rangle+\langle O_2^2(l)\rangle\right)$$

$$-5B_4^0\left(\langle O_4^0(l)\rangle+3\langle O_4^2(l)\rangle\right)$$

$$-\tfrac{21}{2}B_6^0\left(\langle O_6^0(l)\rangle+5\langle O_6^2(l)\rangle\right)\Big\}_l \tag{7.7}$$

$$K_2(T) = \sum_{l}\Big\{\tfrac{35}{8}B_4^0\left(\langle O_4^0(l)\rangle+4\langle O_4^2(l)\rangle+\langle O_4^4(l)\rangle\right)$$

$$+\tfrac{63}{8}B_6^0\left(3\langle O_6^0(l)\rangle+20\langle O_6^2(l)\rangle+5\langle O_6^4(l)\rangle\right)\Big\}_l \tag{7.8}$$

$$K_3(T) = \sum_{l} \Big\{ -\frac{693}{48} B_6^0 \Big(\langle O_6^0(c)\rangle + \frac{15}{2} \langle O_6^2(c)\rangle + 3\langle O_6^4(c)\rangle + \frac{1}{2} \langle O_6^6(c)\rangle \Big) \Big\}_l \tag{7.9}$$

$$K_4(T) = \sum_{l} \Big\{ \frac{1}{16} B_6^6 \Big(\langle O_6^0(c)\rangle + \frac{15}{2} \langle O_6^2(c)\rangle + 3\langle O_6^4(c)\rangle + \frac{1}{2} \langle O_6^6(c)\rangle \Big) \Big\}_l \tag{7.10}$$

In the magnetically ordered phase the magnetoelastic coupling causes a distortion of the hexagonal closed packed structure and other terms than those originating from the anisotropy occur according to the appropriate symmetry. In the frozen lattice model we find the following macroscopic anisotropy constants.

$$\begin{aligned} K_1(T) = \sum_{l} \Big\{ & \langle O_2^0(c)\rangle \Big[-\frac{3}{2} B_2^0 + \frac{3}{2} \big(B_{20}^{\alpha,1} \bar{\varepsilon}^{\alpha,1} + B_{20}^{\alpha,2} \bar{\varepsilon}^{\alpha,2} \big) \\ & \quad + \frac{21}{2} \big(B_{60}^{\alpha,1} \bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2} \bar{\varepsilon}^{\alpha,2} \big) \\ & \quad - \frac{1}{2} B_{22}^{\gamma} \big(\bar{\varepsilon}_1^{\gamma} \cos 2\varphi + \bar{\varepsilon}_2^{\gamma} \sin 2\varphi \big) \Big] + \\ & \langle O_2^2(c)\rangle \Big[-\frac{3}{2} B_2^0 + \frac{3}{2} \big(B_{20}^{\alpha,1} \bar{\varepsilon}^{\alpha,1} + B_{20}^{\alpha,2} \bar{\varepsilon}^{\alpha,2} \big) \\ & \quad + \frac{105}{2} \big(B_{60}^{\alpha,1} \bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2} \bar{\varepsilon}^{\alpha,2} \big) \\ & \quad - \frac{1}{2} B_{22}^{\gamma} \big(\bar{\varepsilon}_1^{\gamma} \cos 2\varphi + \bar{\varepsilon}_2^{\gamma} \sin 2\varphi \big) \Big] + \end{aligned}$$

$$+\langle O_4^0(c)\rangle\Big[-5B_4^0+5\big(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)$$

$$-\tfrac{3}{4}B_{42}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)\Big]+$$

$$\langle O_4^2(c)\rangle\Big[-15B_4^0+15\big(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)$$

$$-4B_{42}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)$$

$$+\tfrac{1}{2}B_{44}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\big)\Big]+$$

$$\langle O_4^4(c)\rangle\Big[-\tfrac{7}{4}B_{42}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)$$

$$+\tfrac{1}{2}B_{44}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\big)\Big]+$$

$$\langle O_6^0(c)\rangle\Big[-\tfrac{21}{2}B_6^0-B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)\Big]+$$

$$\langle O_6^2(c)\rangle\Big[-\tfrac{105}{2}B_6^0-\tfrac{19}{2}B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)$$

$$+\tfrac{15}{4}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\big)\Big]+$$

$$\langle O_6^4(c)\rangle\Big[\tfrac{3}{2}B_6^6\cos 6\varphi-\tfrac{3}{2}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\varphi$$

$$-\tfrac{9}{2}B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\big)$$

$$+\tfrac{13}{2}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\big)\Big]+$$

$$\langle O_6^6(c)\rangle\Big[\tfrac{1}{2}B_6^6\cos 6\varphi-\tfrac{3}{2}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\varphi$$

$$+\tfrac{11}{16}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\big)\Big]\Big\}_{\ell} \qquad (7.11)$$

$$K_2(T) = \sum_{\ell} \Big\{ \langle O_4^0(\iota)\rangle \Big[\tfrac{35}{8} B_4^0 - \tfrac{35}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+ \tfrac{7}{8} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)$$

$$- \tfrac{1}{8} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big] +$$

$$\langle O_4^2(\iota)\rangle \Big[\tfrac{35}{2} B_4^0 - \tfrac{35}{2}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+ \tfrac{7}{2} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)$$

$$- \tfrac{1}{2} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big] +$$

$$\langle O_4^4(\iota)\rangle \Big[\tfrac{35}{8} B_4^0 - \tfrac{35}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+ \tfrac{7}{8} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)$$

$$- \tfrac{1}{8} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big] +$$

$$\langle O_6^0(\iota)\rangle \Big[\tfrac{189}{8} B_6^0 - \tfrac{189}{8}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+ 3 B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)$$

$$- \tfrac{5}{8} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big] +$$

$$\langle O_6^2(\iota)\rangle \Big[\tfrac{315}{2} B_6^0 - \tfrac{315}{2}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$- \tfrac{15}{16} B_6^6 \cos 6\varphi + \tfrac{15}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\varphi$$

$$+ \tfrac{375}{16} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)$$

$$- \tfrac{35}{4} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \sin 4\varphi\right)\Big] +$$

$$
\begin{aligned}
&+\langle O_6^4(c)\rangle\Big[\tfrac{315}{8}B_6^0-\tfrac{315}{8}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)+\\
&\quad\left(-\tfrac{3}{2}B_6^6+\tfrac{3}{2}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\right)\cos 6\varphi\\
&\quad+\tfrac{21}{2}B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)\\
&\quad-\tfrac{67}{8}B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big]+\\
&\langle O_6^6(c)\rangle\Big[\left(-\tfrac{9}{16}B_6^6+\tfrac{9}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\right)\cos 6\varphi\\
&\quad+\tfrac{33}{16}B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)\\
&\quad-\tfrac{11}{4}B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big]\Big\}_{\ell}
\end{aligned}
\tag{7.12}
$$

$$
\begin{aligned}
K_3(T)=\sum_{\ell}\Big\{&\langle O_6^0(c)\rangle\Big[-\tfrac{693}{48}B_6^0+\tfrac{693}{48}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\\
&\quad-\tfrac{33}{16}B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)\\
&\quad+\tfrac{11}{16}B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big]+\\
&\langle O_6^2(c)\rangle\Big[-\tfrac{15}{2}\cdot\tfrac{693}{48}B_6^0+\tfrac{15}{2}\cdot\tfrac{693}{48}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\\
&\quad-\tfrac{33}{16}\tfrac{15}{2}B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)\\
&\quad+\tfrac{165}{32}B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big]+\\
&\langle O_6^4(c)\rangle\Big[-\tfrac{693}{16}B_6^0+\tfrac{693}{16}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\\
&\quad-\tfrac{99}{16}B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi+\bar{\varepsilon}_2^{\gamma}\sin 2\varphi\right)\\
&\quad+\tfrac{33}{16}B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi+\bar{\varepsilon}_2^{\gamma}\sin 4\varphi\right)\Big]+
\end{aligned}
$$

$$+ \langle O_6^0(c)\rangle\Big[-\tfrac{693}{96}B_6^0 + \tfrac{693}{16}(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})$$
$$-\tfrac{33}{32}B_{62}^{\gamma}(\bar{\varepsilon}_1^{\gamma}\cos 2\varphi + \bar{\varepsilon}_2^{\gamma}\sin 2\varphi)$$
$$+\tfrac{11}{32}B_{64}^{\gamma}(\bar{\varepsilon}_1^{\gamma}\cos 4\varphi + \bar{\varepsilon}_2^{\gamma}\sin 4\varphi)\Big]\Big\}_{\ell} \tag{7.13}$$

$$K_4(T) = \sum_{\ell}\Big\{\langle O_6^0(c)\rangle\Big[\tfrac{1}{16}B_6^6 - \tfrac{1}{16}(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})\Big] +$$
$$\langle O_6^2(c)\rangle\Big[\tfrac{15}{32}B_6^6 - \tfrac{15}{32}(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})\Big] +$$
$$\langle O_6^4(c)\rangle\Big[\tfrac{3}{16}B_6^6 - \tfrac{3}{16}(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})\Big] +$$
$$\langle O_6^6(c)\rangle\Big[\tfrac{1}{32}B_6^6 - \tfrac{1}{32}(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})\Big]\Big\}_{\ell} \tag{7.14}$$

All φ-dependent terms of $K_1(T)$, $K_2(T)$ and $K_3(T)$ are excluded if only the hexagonal terms are considered.

The temperature dependence is expressed through the thermal mean values of the Stevens operators that have been calculated in section 4. Besides the *equilibrium strains are given as function of temperature* through the Stevens operator thermal mean values, also calculated in section 4.

In appendix 9 it is shown that the anisotropy constants defined in equation (7.2) are related to the anisotropy coefficients defined by the equation

$$\mathcal{F}(\theta,\varphi) = \mathcal{K}_{0,0}(T) + \mathcal{K}_{2,0}(T)P_2^0(\cos\theta) + \mathcal{K}_{4,0}(T)P_4^0(\cos\theta)$$
$$+\mathcal{K}_{6,0}(T)P_6^0(\cos\theta) + \mathcal{K}_{6,6}(T)\sin^6\theta\cos 6\varphi$$
$$+ \cdots \tag{7.15}$$

through the relations

$$\mathcal{H}_{0,0}(T) = \frac{2}{105}\left(35K_1(T) + 28K_2(T) + 24K_3(T)\right) \tag{7.16}$$

$$\mathcal{H}_{2,0}(T) = -\frac{2}{21}\left(7K_1(T) + 8K_2(T) + 8K_3(T)\right) \tag{7.17}$$

$$\mathcal{H}_{4,0}(T) = \frac{8}{385}\left(11K_2(T) + 18K_3(T)\right) \tag{7.18}$$

$$\mathcal{H}_{6,0}(T) = -\frac{16}{231}\, K_3(T) \tag{7.19}$$

$$\mathcal{H}_{6,0}(T) = K_4(T) \tag{7.20}$$

A review of the status of temperature dependence of the magneto crystalline anisotropy has been given by Callen and Callen[27] in 1966. Since then a number of authors have dealt with the object Brooks, Goodings and Ralph[32], Brooks[33], Brooks[34], Egami[35], Brooks and Egami[36]. They have extended the simple K(K+1)/2 law taking into account the non-cylindrical anisotropy by introducing a single ellipticity parameter describing the non- circular spin precession. They have found that the axial anisotropy (q=0) is corrected linear by the ellipticity parameter in contrast to the result of equation (4.59) where we have shown that the axial anisotropy is corrected by the ellipticity parameter squared. Besides they have not been able to set up relations for the different non-axial anisotropy (q=2, q=4) as carried out in the equations (4.60) and (4.61). Finally they have not taken into account that the anisotropy constants are linear conbinations of axial anisotropy terms as well as non--axial anisotropy terms as has been included in the relations (7.7)-(7.10) and (7.11)-(7.14).

8. A NUMERICAL CALCULATION OF THE TEMPERATURE DEPENDENCE OF THE MACROSCOPIC ANISOTROPY CONSTANTS OF TERBIUM

8.1. Introduction

In this section we carry out a numerical calculation of the temperature dependence of the macroscopic anisotropy constants of terbium based on the formulae set up in section 4 and section 7 and inelastic neutron scattering experiments done by Bjerrum-Møller, Houmann, Nielsen and Mackintosh[37].

8.2. The Temperature Dependence of the Stevens Operators

The temperature dependence of the Stevens operators has in section 4 been expressed by the two characteristic functions $\Delta M(T)$ and $b(T)$. The relative magnetization $m(T)$ is connected with $\Delta M(T)$ through the relation

$$m(T) = \frac{M(T)}{M(0)} = 1 - \Delta M(T) \tag{8.1}$$

where $M(T)$ is the magnetization at temperature T and $M(0)$ the magnetization at $T = 0\ ^{\circ}K$. However as is seen from the calculations in appendix 6 zero point motion is explicitely taken into account. Therefore we find the zero point corrected, relative magnetization to

$$m'(T) = \frac{m(T)}{m(0)} = 1 - \frac{\Delta M(T) - \Delta M(0)}{m(0)} \tag{8.2}$$

where $m(0) = 1 - \Delta M(0)$ is the relative magnetization at $T = 0^{\circ}K$ and $\Delta M(0) = 0.00208$ for Tb. For terbium it is found that model no. 2 gives the best fit to the experimental obtained spin wave dispersion relations at $T = 4.2^{\circ}K$. The relative magnetization of Tb is found to agree with the measured magnetization curve obtained by Hegland, Legvold and Spedding[38]. The calculated and measured curves are compared in fig. 1. The calculation of the ellipticity parameter $b(T)$ as a function of temperature also include zero point motion. The temperature dependence is shown in fig. 2. The zero point value of $b(T)$ is $b(0) = -0.00484$.

By means of the two characteristic functions $\Delta M(T)$ and $b(T)$ the temperature dependence of the Stevens operators has been calculated. The results that are shown in fig. 3, fig. 4 and fig. 5 are normalized in the following way

$$\langle O_K^q(c)\rangle_T / \langle O_K^q(c)\rangle_{T=0} \tag{8.3}$$

where the zero temperature values are

$$\langle O_2^0(c)\rangle_{T=0} = 6.559\ 10^{1}\ ;\ \langle O_2^2(c)\rangle_{T=0} = -3.315\ 10^{-1}$$

$$\langle O_4^0(c)\rangle_{T=0} = 5.821\ 10^{3}\ ;\ \langle O_4^2(c)\rangle_{T=0} = -4.410\ 10^{1}$$

$$\langle O_6^0(c)\rangle_{T=0} = 1.596\ 10^{5}\ ;\ \langle O_6^2(c)\rangle_{T=0} = -1.609\ 10^{3}$$

$$\langle O_4^4(c)\rangle_{T=0} = 2.756\ 10^{-1}\ ;\ \langle O_6^4(c)\rangle_{T=0} = 3.858\ 10^{1}$$

As $\langle O_l^4(c)\rangle$ is proportional to b(T) squared the normalized curve is the same for $\langle O_4^4(c)\rangle$ and $\langle O_6^4(c)\rangle$.

8.3. The Crystal Field Parameters of Terbium

The crystal field parameters of terbium have been calculated by means of a point charge model, Danielsen[23]. In a notation after Hutchings[9] the crystal field parameters are given by

$$B_l^m = A_l^m \langle r^l\rangle\, \theta_l \tag{8.4}$$

Here the θ_l are the Stevens coefficients which are the proportionality coefficients of the Stevens operator equivalents transformation. For terbium they are after Elliott and Stevens[39]

$$\theta_2 = -1.010\ 10^{-2}$$

$$\theta_4 = 1.224\ 10^{-4}$$

$$\theta_6 = -1.12\ 10^{-6}$$

$\langle r^l\rangle$ denotes the mean value of the n^{th} power of the radial distance of the 4f wave functions. They have been calculated by Freeman and Watson[40] and they found for terbium

$$\langle r^2 \rangle = 0.756 \text{ a.u.} = 0.2116 \; 10^{-16} \text{ cm}^2$$

$$\langle r^4 \rangle = 1.42 \text{ a.u.} = 0.1112 \; 10^{-32} \text{ cm}^4$$

$$\langle r^6 \rangle = 5.69 \text{ a.u.} = 0.0349 \; 10^{-48} \text{ cm}^6$$

(1 a.u. = 0.529 10^{-8} cm).

The A_l^m are here found by summing over nearest and next nearest neighbours. The crystal field parameters are therefore dependent of the lattice parameters. By means of measurements of the magnetostriction by Rhyne and Legvold[41] and of the lattice parameters by Darnell[42] the temperature dependence of the crystal field parameters has been calculated. These calculations are shown in fig. 6, fig. 7, fig. 8 and fig. 9. In an ideal hexagonal closed packed structure B_4^o, B_6^o and B_6^6 are the only finite parameters. In a hcp lattice with c/a different from the ideal value $\sqrt{8/3}$ the B_2^o is also present. However, in terbium magnetostriction is effective in the ordered region, which means for temperature lower than 228^{o}K, Elliott[43]. The magnetostrictive coupling causes the crystal field parameters B_2^2, B_4^2, B_4^4, B_6^2 and B_6^4 to be finite. This has been shown theoretically by Danielsen[23]. Besides the magnetostriction modify the unstrained crystal field parameter B_2^o, B_4^o, B_6^o and B_6^6. At the figures, showing the temperature dependence of the crystal field parameters, it is seen that the magnetostriction dependent crystal field parameters vanish at T = 228^{o}K, whereas the unstrained parameters B_2^o, B_4^o, B_6^o and B_6^6 are finite in the paramegnetic region. The crystal field parameters are given in milli electron volts.

8.4. The Macroscopic Anisotropy Coefficients of Terbium

The temperature dependent macroscopic anisotropy constants are found from the formulae (7.11) - (7.14). The formulae (7.17) - (7.20) connect the anisotropy constants and the anisotropy coefficients. In fig. 10, fig. 11, fig. 12 and fig. 13 the temperature dependence of the macroscopic anisotropy coefficients are calculated by means of crystal field parameters calculated in the point charge approximation. The coefficients are given in milli electron volts or in ergs/cm^3. For terbium we have at T = 0^{o}K

1 mev/atom = 5.06642 10^7 ergs/cm^3

The calculated macroscopic anisotropy coefficients are at T = 0^0K

$\varkappa_{2.0}(0)$ = 3.5461 mev/atom = 1.7966 10^8 ergs/cm^3

$\varkappa_{4.0}(0)$ = -0.5989 mev/atom = -0.3034 10^8 ergs/cm^3

$\varkappa_{6.0}(0)$ = -9.2434 10^{-3} mev/atom = - 4.6831 10^5 ergs/cm^3

$\varkappa_{6.6}(0)$ = 5.1263 10^{-3} mev/atom = 2.5972 10^5 ergs/cm^3

The macroscopic anisotropy coefficients have been measured by different methods. In the following scheme we have gathered these experimental values of the anisotropy coefficients for terbium.

$\varkappa_{2.0}$	$\varkappa_{4.0}$	$\varkappa_{6.0}$	$\varkappa_{6.6}$	T	Method	Ref. no.
ergs/cm^3	ergs/cm^3	ergs/cm^3	ergs/cm^3	^{0}K	-	-
5.65 10^8	4.6 10^7		1.85 10^6	4	differential torque method	44
5.5 10^8			2.42 10^6	4	torque measurement	45 46
3.1 10^8				0	ferromagnetic resonance	47
2.6 10^8	6.3 10^7	4.4 10^7		4	torque magnetometer	48
2.7 10^8				105	torque method in pulsed magnetic field	49
			2.2 10^6	0	torque magnetometer	50
			2.9 10^6	0	torque measurements	51
1.8 10^8	-3.0 10^7	-4.7 10^5	2.6 10^5	0	theoretical values	

It is seen that the theoretical calculated values of $\varkappa_{2.0}$ and $\varkappa_{4.0}$ are of right order, but the sign of $\varkappa_{4.0}$ disagree with the theoretical prediction from the point charge calculation. The theoretical values of $\varkappa_{6.0}$ and $\varkappa_{6.6}$ are of lower order than the experimental obtained values of the anisotropy coefficients and the sign of $\varkappa_{6.0}$ disagree with the theoretical prediction.

However, the point charge model calculation only gives an estimate of the crystal field parameters as this theory neglects the contribution of the conduction electrons to the crystalline electric field. Therefore to make a comparison of the theoretical calculated temperature dependence of the anisotropy coefficients with experiments we might take the crystal field parameters as adjustable parameters. In fig. 14, fig. 15 and fig. 16 we have, however, only scaled the theoretical zero temperature values of the anisotropy coefficients with the experimental values obtained by Feron et. al. [44]. We find a good agreement between experimental and theoretical values of $\kappa_{2,0}$ and $\kappa_{4,0}$ but less good agreement between the $\kappa_{6,6}$ values.

SUMMARY

By means of the operator equivalents method we have in chapter 2 calculated an expression of the Racah operator, $\tilde{O}_{K,q}$ with maximum q-value, namely q=K. From this relation the complete set of Racah operators has been generated for all values of K up to K=8. Further has the commutator relation of two non-commuting Racah operators been established. Finally in this section the connection between the Stevens operators and the Racah operators has been set up. Requiring the matrix elements between corresponding states to be identical we have in chapter 3 calculated well ordered Bose operator expansions of the Racah operators and of the Stevens operators. It has been shown for tensor operators of rank one that this method of matching matrix elements corresponds with the Holstein-Primakoff method of transforming angular momentum operators to Bose operators. Introducing an ellipticity parameter, b(T) that accounts for the non-circular spin precession about the direction of magnetization the well known K(K+1)/2 low temperature law of the magnetic anisotropy coefficients has in chapter 4 been extended by setting up explicit expressions of the temperature dependence of the non-axial anisotropy coefficients. The correspondence with the K(K+1)/2 law in the limit b(T) = 0 has been shown. The temperature dependence of the magnon energy gap has been established by means of a spin wave calculation in chapter 5 as well as by a calculation based on ferromagnetic resonance theory in chapter 6. The result of the spin wave calculation has been expressed as a power law in the relative magnetization, m(T) and a term containing the ellipticity parameter, b(T). The m(T)-dependence has been written out explicitely taking into account all single ion anisotropy terms as well as all single ion magnetostriction terms of the Hamiltonian of the heavy rare earths that have hexagonal crystal symmetry. Using the results from chapter 4 of the temperature dependence of the Stevens operators the resonans theory calculation of the temperature dependence of the energy gap gives the same dependence of the relative magnetization as do the spin wave calculation in chapter 5. By means of the spin wave dispersion relation of terbium measured at 4.2°K by inelastic neutron scattering experiments we have calculated the magnetization curve of terbium and have found good agreement with the experimental obtained magnetization curve. Besides the relative magnetization the ellipticity parameter of terbium has been calculated making it possible together with a point charge model calculation of the crystal field parameters to calculate the temperature dependence of the macroscopic anisotropy coefficients. We have found, taking into account the limitations of the point charge model, a fairly good agreement with experiments.

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APPENDICES

Appendix 1: The Reduced Matrix Element of a Racah Operator

The matrix element of a Racah operator within a manifold of given angular momentum J is

$$\langle J m | \tilde{O}_{K,q} | J m' \rangle = (-1)^{J-m} \begin{pmatrix} J & K & J \\ -m & q & m' \end{pmatrix} \langle J \| \tilde{O}_K \| J \rangle$$

(A 1.1)

From this equation we find for the reduced matrix element $\langle J \| \tilde{O}_K \| J \rangle$:

$$\langle J \| \tilde{O}_K \| J \rangle = \frac{\langle J m | \tilde{O}_{K,q} | J m' \rangle}{(-1)^{J-m} \begin{pmatrix} J & K & J \\ -m & q & m' \end{pmatrix}} \qquad \text{(A 1.2)}$$

To calculate the reduced matrix element we choose special values of m, q and m', namely

$$m = J$$
$$q = k$$
$$m' = J - K$$

From (2.9) we know that

$$\tilde{O}_{KK} = \frac{(-1)^K}{2^K K!} \sqrt{(2K)!}\,(J^+)^K$$

using $J^+ | J\, m\rangle = \sqrt{(J - m)(J + m + 1)}\, | J\, m + 1\rangle$, Edmonds[3]
we find

$$\langle J J | \tilde{O}_{KK} | J\, J-K \rangle = \frac{(-1)^K}{2^K K!} \sqrt{(2K)!}\, \langle J J | (J^+)^K | J\, J-K \rangle$$

$$= \frac{(-1)^K}{2^K K!} \sqrt{(2K)!} \sqrt{K! \frac{(2J)!}{(2J-K)!}}$$

$$= \frac{(-1)^K}{2^K K!} \sqrt{\frac{K!\,(2K)!\,(2J)!}{(2J-K)!}} \qquad \text{(A 1.3)}$$

The 3j-symbol is defined by, Rothenberg et al[12)]

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} \frac{1}{\sqrt{2j_3+1}} \left(j_1 m_1 j_2 m_2 \mid j_1 j_2 j_3 - m_3 \right) \tag{A 1.4}$$

Here we put:

$$j_1 = j_3 = J \; ; \quad j_2 = K$$

$$m_1 = -J \; ; \quad m_2 = K \; ; \quad m_3 = J-K$$

$$\begin{pmatrix} J & K & J \\ -J & K & J-K \end{pmatrix} = \begin{pmatrix} K & J & J \\ K & J-K & -J \end{pmatrix} = (-1)^K \frac{1}{\sqrt{2J+1}} \left(K K J J-K \mid K J J J \right)$$

The Vector coupling coefficient (the Clebsh-Gordan coefficient) is calculated by the formula, Edmonds[3)].

$$\left(j_1 j_1 j_2 \, m-j_1 \mid j_1 j_2 j \, m \right) =$$

$$\sqrt{\frac{(2j+1)\ (2j_1)!\ (-j_1+j_2+j)!\ (j_1+j_2-m)!\ (j+m)!}{(j_1+j_2-j)!\ (j_1-j_2+j)!\ (j_1+j_2+j+1)!\ (-j_1+j_2+m)!\ (j-m)!}}$$

Now putting

$$j_1 = K \; ; \quad j_2 = J \; ; \quad j = J \; ; \quad m = J$$

$$\left(K K J J-K \mid K J J J \right) = \sqrt{\frac{(2J+1)(2K)!\ (2J-K)!\ K!\ (2J)!}{K!\ K!\ (2J+K+1)!\ (2J-K)!}}$$

$$= \sqrt{\frac{(2K)!\ (2J+1)!}{K!\ (2J+K+1)!}}$$

so the 3-j symbol becomes

$$\begin{pmatrix} J & K & J \\ -J & K & J-K \end{pmatrix} = \frac{(-1)^K}{\sqrt{2J+1}} \sqrt{\frac{(2J+1)\,(2J)!\,(2K)!}{K!\,(2J+K+1)!}}$$

$$= (-1)^K \sqrt{\frac{(2J)!\,(2K)!}{K!\,(2J+K+1)!}} \qquad \text{(A 1.5)}$$

Now we find for the reduced matrix element:

$$\langle J \| \tilde{O}_K \| J \rangle = \frac{\langle J\,J \,|\, \tilde{O}_{KK} \,|\, J\;J-K \rangle}{\begin{pmatrix} J & K & J \\ -J & K & J-K \end{pmatrix}}$$

$$= \frac{\dfrac{(-1)^K}{2^K K!} \sqrt{\dfrac{K!\,(2K)!\,(2J)!}{(2J-K)!}}}{(-1)^K \sqrt{\dfrac{(2J)!\,(2K)!}{K!\,(2J+K+1)!}}}$$

$$\langle J \| \tilde{O}_K \| J \rangle = \frac{1}{2^K} \sqrt{\frac{(2J+K+1)!}{(2J-K)!}} \qquad \text{(A 1.6)}$$

Appendix 2: The commutator of two non-commuting Racah operators

Two Racah operators acting on the same dynamic variable, i, within a manifold of given angular momentum J do not commute. From the matrix formulation of quantum mechanics we have for an operator acting on an eigenfunction: $\hat{A}|s\rangle = \sum_i |i\rangle\langle i|\hat{A}|s\rangle$. For the non-commuting Racah operators $\tilde{O}_{K_1q_1}(i)$ and $\tilde{O}_{K_2q_2}(i)$ we set up the following relations:

$$\tilde{O}_{K_2q_2}(i)|Jm\rangle = \sum_{m'} |Jm'\rangle\langle Jm'|\tilde{O}_{K_2q_2}(i)|Jm\rangle$$

$$= \sum_{m'} (-1)^{J-m'} \begin{pmatrix} J & K_2 & J \\ -m' & q_2 & m \end{pmatrix} \langle J\|\tilde{O}_{K_2}(i)\|J\rangle |Jm'\rangle \tag{A 2.1}$$

and

$$\tilde{O}_{K_1q_1}(i)|Jm'\rangle = \sum_{m''} |Jm''\rangle\langle Jm''|\tilde{O}_{K_1q_1}(i)|Jm'\rangle$$

$$= \sum_{m''} (-1)^{J-m''} \begin{pmatrix} J & K_1 & J \\ -m'' & q_1 & m' \end{pmatrix} \langle J\|\tilde{O}_{K_1}(i)\|J\rangle |Jm''\rangle \tag{A 2.2}$$

using (2.11) for the matrix element of a Racah operator. As the operators are both acting on the same dynamic variable we find

$$\tilde{O}_{K_1q_1}(i)\,\tilde{O}_{K_2q_2}(i)|Jm\rangle =$$

$$\sum_{m'm''} (-1)^{2J-m'-m''} \begin{pmatrix} J & K_1 & J \\ -m'' & q_1 & m' \end{pmatrix} \begin{pmatrix} J & K_2 & J \\ -m' & q_2 & m \end{pmatrix} \times$$

$$\cdot \langle J\|\tilde{O}_{K_1}(i)\|J\rangle\langle J\|\tilde{O}_{K_2}(i)\|J\rangle |Jm''\rangle \tag{A 2.3}$$

The following formula combining 3j -and 6j-symbols are now used, Rothenberg[12])

$$\sum_{m_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_3 & l_1 & l_2 \\ -m_3 & n_1 & n_2 \end{pmatrix} =$$

$$\sum_{l_3 n_3} (-1)^{j_3 + l_3 + m_1 + n_1} (2l_3+1) \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ n_1 & m_2 & n_3 \end{pmatrix} \begin{pmatrix} l_3 & j_1 & l_2 \\ -n_3 & m_1 & n_2 \end{pmatrix} \tag{A 2.4}$$

with the symbols

$$j_1 = j_3 = l_2 = J \; ; \quad j_2 = K_1 \; ; \quad l_1 = K_2 \; ; \quad l_3 = K_3$$

$$m_1 = -m'' \; ; \; m_2 = q_1 \; ; \; m_3 = m' \; ; \; n_1 = q_2 \; ; \; n_2 = m \; ; \; n_3 = q_3$$

$$\sum_{m'} \begin{pmatrix} J & K_1 & J \\ -m'' & q_1 & m' \end{pmatrix} \begin{pmatrix} J & K_2 & J \\ -m' & q_2 & m \end{pmatrix} =$$

$$\sum_{K_3 q_3} (-1)^{J + K_3 - m'' + q_2} (2K_3+1) \begin{Bmatrix} J & K_1 & J \\ K_2 & J & K_3 \end{Bmatrix} \begin{pmatrix} K_2 & K_1 & K_3 \\ q_2 & q_1 & q_3 \end{pmatrix} \begin{pmatrix} K_3 & J & J \\ -q_3 & -m'' & m \end{pmatrix}$$

$$= \sum_{K_3 q_3} (-1)^{\alpha} (2K_3+1) \begin{Bmatrix} K_1 & K_2 & K_3 \\ J & J & J \end{Bmatrix} \begin{pmatrix} K_1 & K_2 & K_3 \\ q_1 & q_2 & q_3 \end{pmatrix} \begin{pmatrix} J & K_3 & J \\ -m'' & -q_3 & m \end{pmatrix} \tag{A 2.5}$$

with $\quad \alpha = J + K_3 - m'' + q_2 + (K_1 + K_2 + K_3) + (2J + K_3)$

using the odd-permutation rule for 3j-symbols

$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix}$ and the fact that a 6j-symbol remains an invariant under interchange of columns and at interchange of any two numbers in the bottom row with the corresponding two numbers in the top row.

Now the total exponent is considered, namely

$$2J-m'-m''+\alpha = 2J-m'-m''+J+k_3-m''+q_2+(k_1+k_2+k_3)+(2J+k_3)$$

$$(-1)^{2J-m'-m''+\alpha} = (-1)^{k_1+k_2+k_3}(-1)^{4J}(-1)^{2k_3}(-1)^{J-m''}(-1)^{q_2-m'-m''}$$

$(-1)^{4J} = 1$ for J integer and J half integer

$(-1)^{2K_3} = 1$ for K_3 integer, and K_3 really is integer for a Racah operator

'rom the 3j-symbol to the left in (A 2.5) we find $m'' = q_1 + m'$ and from the j-symbol

$\begin{pmatrix} K_1 & K_2 & K_3 \\ q_1 & q_2 & q_3 \end{pmatrix}$ we have $q_1 + q_2 + q_3 = 0$ for which reason

$$(-1)^{q_2-m'-m''} = (-1)^{q_2-m''-(m''-q_1)} = (-1)^{q_1+q_2}(-1)^{-2m''}$$

$$= (-1)^{-q_3} = (-1)^{q_3}$$

ıs $(-1)^{-2m''} = (-1)^{2m''} = 1$

or m'' integer, and m'' is really an integer for the Racah operators.

'he resulting exponent:

$$(-1)^{2J-m'-m''+\alpha} = (-1)^{k_1+k_2+k_3}(-1)^{J-m''}(-1)^{q_3} \qquad \text{(A 2.6)}$$

ınd for the two Racah operators acting on $|Jm\rangle$ we therefore find

$$\tilde{O}_{k_1q_1}(i)\,\tilde{O}_{k_2q_2}(i)\,|Jm\rangle = \sum_{k_3q_3}(-1)^{k_1+k_2+k_3}(2k_3+1)\begin{Bmatrix} k_1 & k_2 & k_3 \\ J & J & J \end{Bmatrix}\begin{pmatrix} k_1 & k_2 & k_3 \\ q_1 & q_2 & q_3 \end{pmatrix}\cdot$$

$$\times \langle J\|\tilde{O}_{k_1}(i)\|J\rangle\langle J\|\tilde{O}_{k_2}(i)\|J\rangle \times$$

$$\times \sum_{m''}(-1)^{J-m''}(-1)^{q_3}\begin{pmatrix} J & k_3 & J \\ -m'' & -q_3 & m \end{pmatrix}|Jm''\rangle$$

(A 2.7)

r

$$\tilde{O}_{K_1q_1}(i)\,\tilde{O}_{K_2q_2}(i) = \sum_{K_3q_3}(-1)^{K_1+K_2+K_3}(2K_3+1)\begin{Bmatrix}K_1 & K_2 & K_3\\ J & J & J\end{Bmatrix}\begin{pmatrix}K_1 & K_2 & K_3\\ q_1 & q_2 & q_3\end{pmatrix}$$

$$\times\frac{\langle J\|\tilde{O}_{K_1}(i)\|J\rangle\langle J\|\tilde{O}_{K_2}(i)\|J\rangle}{\langle J\|\tilde{O}_{K_3}(i)\|J\rangle}\,O^{+}_{K_3q_3}(i)$$

(A 2.8)

where we have used that $\tilde{O}^{+}_{K_3,q_3} = (-1)^{q_3}\tilde{O}_{K_3-q_3}$. When forming the product $\tilde{O}_{K_2q_2(i)}\tilde{O}_{K_1q_1(i)}$ everything is unchanged except the 3j-symbol where we find $\begin{pmatrix}K_2 & K_1 & K_3\\ q_2 & q_1 & q_3\end{pmatrix} = (-1)^{K_1+K_2+K_3}\begin{pmatrix}K_1 & K_2 & K_3\\ q_1 & q_2 & q_3\end{pmatrix}$
From this we immediately find the commutator relation as $(-1)^{2(K_1+K_2+K_3)} = 1$ for the K's integers, which they infact are for Racah operators.

$$[\tilde{O}_{K_1q_1}(i), \tilde{O}_{K_2q_2}(i)] = \sum_{K_3q_3}\{(-1)^{K_1+K_2+K_3}-1\}\,(2K_3+1)\begin{Bmatrix}K_1 & K_2 & K_3\\ J & J & J\end{Bmatrix}\begin{pmatrix}K_1 & K_2 & K_3\\ q_1 & q_2 & q_3\end{pmatrix}$$

$$\times\frac{\langle J\|\tilde{O}_{K_1}(i)\|J\rangle\langle J\|\tilde{O}_{K_2}(i)\|J\rangle}{\langle J\|\tilde{O}_{K_3}(i)\|J\rangle}\,\tilde{O}^{+}_{K_3q_3}(i)$$

(A 2.9)

where the reduced matrix element is given by
(appendix 1): $\langle J\|\tilde{O}_K\|J\rangle = \frac{1}{2^K}\sqrt{\frac{(2J+K+1)!}{(2J-K)!}}$

As a check of the commutator relation calculted we now demonstrate that it is consistent with the definition equations of the Racah operators,

$$[J_z, \tilde{O}_{K,q}] = q\,\tilde{O}_{K,q} \qquad ((2.5))$$

$$[J^{\pm}, \tilde{O}_{K,q}] = [K(K+1)-q(q\pm1)]^{1/2}\,\tilde{O}_{K,q\pm1} \qquad ((2.6))$$

<u>Case 1</u>

<u>$K_1 = 1,\ q_1 = 0 \ : \tilde{O}_{K_1,q_1} = \tilde{O}_{1,0} = J_z$</u>

From the commutator relation we find

$$[J_z, \tilde{O}_{K_2 q_2}] = \sum_{K_3 q_3} \{(-1)^{1+K_2+K_3} - 1\} (2K_3+1) \begin{Bmatrix} 1 & K_2 & K_3 \\ J & J & J \end{Bmatrix} \begin{pmatrix} 1 & K_2 & K_3 \\ 0 & q_2 & q_3 \end{pmatrix} \times$$
$$\times \frac{\langle J \| \tilde{O}_1 \| J \rangle \langle J \| \tilde{O}_{K_2} \| J \rangle}{\langle J \| \tilde{O}_{K_3} \| J \rangle} \tilde{O}^{\dagger}_{K_3 q_3}$$

(A 2.10)

$(-1)^{1+K_2+K_3} - 1 \neq 0 \Rightarrow 1+K_2+K_3$ odd $\Rightarrow K_2+K_3$ even

The 3j-symbol gives the triangle conditions:

$1+K_2-K_3 \quad 0$
$1-K_2+K_3 \quad 0$
$-1+K_2+K_3 \quad 0$, and given are $K_2 \quad 0,\ K_3 \quad 0$

one of these, namely $1 \cdot K_2-K_3$ gives as an example

a) $K_2-K_3 = 1 \Rightarrow$ one even <u>and</u> the other odd
b) $K_2-K_3 = 0 \Rightarrow$ both even <u>or</u> both odd

which means: $K_2 = K_3 = K$

Further from the 3j-symbol:

$0 + q_2 + q_3 = 0 \Rightarrow q_2 = -q_3 = q$

so we find for the commutator

$$[J_z, \tilde{O}_{K,q}] = (-2)(2K+1) \begin{pmatrix} 1 & K & K \\ 0 & q & -q \end{pmatrix} \begin{Bmatrix} 1 & K & K \\ J & J & J \end{Bmatrix} \langle J \| \tilde{O}_1 \| J \rangle \tilde{O}^{\dagger}_{K,-q}$$

(A 2.11)

From Edmonds[3)] we have for the 3j-symbol

$$\begin{pmatrix} 1 & K & K \\ 0 & q & -q \end{pmatrix} = \begin{pmatrix} K & K & 1 \\ q & -q & 0 \end{pmatrix} = (-1)^{K-q} \frac{q}{\sqrt{K(2K+1)(K+1)}} \quad \text{(A 2.12)}$$

From appendix 1 the reduced matrix element

$$\langle J \| \tilde{O}_1 \| J \rangle = \frac{1}{2}\sqrt{\frac{(2J+2)!}{(2J-1)!}} \tag{A 2.13}$$

From (2.10) we have

$$\tilde{O}^{\dagger}_{K,-q} = (-1)^{q}\,\tilde{O}_{K,q} \tag{A 2.14}$$

For the 6j-symbol we find from Rothenberg[12]:

$$\begin{Bmatrix} 1 & K & K \\ J & J & J \end{Bmatrix} = (-1)^{1+K+2J}\sqrt{\frac{(2J-1)!}{(2J+2)!}}\; 2K(K+1)\frac{1}{\sqrt{2K(2K+1)(2K+2)}} \tag{A 2.15}$$

The commutator now becomes

$$[J_z, \tilde{O}_{K,q}] = (-2)(2K+1)(-1)^{K+q}\frac{q}{\sqrt{K(2K+1)(K+1)}}(-1)^{K+1}\sqrt{\frac{(2J-1)!}{(2J+2)!}}$$

$$\cdot\, 2K(K+1)\cdot\frac{1}{\sqrt{2K(2K+1)(2K+2)}}\,\frac{1}{2}\sqrt{\frac{(2J+2)!}{(2J-1)!}}\,(-1)^{q}\tilde{O}_{K,q}$$

$$= q\,\tilde{O}_{K,q} \tag{A 2.16}$$

which is one the definition equations of the Racah operators.

Case 2

$K_1 = 1,\ q_1 = 1 \ :\ \tilde{O}_{K_1,q_1} = \tilde{O}_{1,1} = -\frac{1}{\sqrt{2}}J^{+}$

Using these values we find for the commutator:

$$\left[-\frac{1}{\sqrt{2}}J^{+}, \tilde{O}_{K_2 q_2}\right] = \sum_{K_3 q_3}\left\{(-1)^{1+K_2+K_3} - 1\right\}(2K_3+1)\begin{pmatrix} 1 & K_2 & K_3 \\ 1 & q_2 & q_3 \end{pmatrix}\begin{Bmatrix} 1 & K_2 & K_3 \\ J & J & J \end{Bmatrix}$$

$$\cdot\,\frac{\langle J\|\tilde{O}_1\|J\rangle\langle J\|\tilde{O}_{K_2}\|J\rangle}{\langle J\|\tilde{O}_{K_3}\|J\rangle}\,\tilde{O}^{\dagger}_{K_3 q_3} \tag{A 2.17}$$

from case 1 we have: $K_2 = K_3 = K$
from the 3j-symbol:
$1+q_2+q_3 = 0 \Rightarrow q_3 = -(q_2+1) ; q_2 = q$
for which reason

$$[J^+, \tilde{O}_{K,q}] = (-\sqrt{2})(-2)(2K+1)\langle J\|\tilde{O}_1\|J\rangle \begin{Bmatrix} 1 & K & K \\ J & J & J \end{Bmatrix} \begin{pmatrix} 1 & K & K \\ 1 & q & -(q+1) \end{pmatrix} \tilde{O}^+_{K,-(q+1)} \qquad \text{(A 2.18)}$$

From Edmonds[3] we find the 3j-symbol

$$\begin{pmatrix} 1 & K & K \\ 1 & q & -(q+1) \end{pmatrix} = (-1)^{K-q} \sqrt{\frac{(K-q)(K+q+1)\cdot 2}{(2K+2)(2K+1)\,2K}} \qquad \text{(A 2.19)}$$

and from equation (2.10) we find

$$\tilde{O}^+_{K,-(q+1)} = (-1)^{q+1}\,\tilde{O}_{K,q+1}$$

The 6j-symbol and the reduced matrix element have been calculated under case 1. Therefore the commutator becomes:

$$[J^+, \tilde{O}_{K,q}] = (-\sqrt{2})(-2)(2K+1)\,\frac{1}{2}\sqrt{\frac{(2J+2)!}{(2J-1)!}}\,(-1)^{K+1}\sqrt{\frac{(2J-1)!}{(2J+2)!}}$$

$$\times \frac{2K(K+1)}{\sqrt{2K(2K+1)(2K+2)}} \times (-1)^{K-q}\sqrt{\frac{(K-q)(K+q+1)\cdot 2}{(2K+2)(2K+1)\,2K}}$$

$$\times (-1)^{q+1}\,\tilde{O}_{K,q+1}$$

$$= \sqrt{K(K+1)-q(q+1)}\;\;\tilde{O}_{K,q+1} \qquad \text{(A 2.20)}$$

which is the definition equation of a Racah operator commutated by J^+. An analogue and straightforward calculation can be performed for the $[J^-, \tilde{O}_{K,q}]$ commutator.

APPENDIX 3

The Coefficients of the Well-ordered Bose Operator Expansions of the Racah Operators

The Racah operators are expanded in Bose operators as given by formula (3.32)

$$\tilde{O}_{K,q} = \left(A^K_{q,0} + A^K_{q,1} a^+ a + A^K_{q,2} a^+ a^+ a a + \cdots \right) a^q \qquad \text{(A 3.1)}$$

Using the idea of requiring the correct matrix elements between the ground state and the first excited state we found in section (3.3) for the expansion coefficients

$$A^K_{q,n} = \sqrt{\frac{1}{n!(n+q)!}}(-1)^n \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J+n & q & J-(n+q) \end{pmatrix}$$
$$- \left(\frac{1}{n!} A^K_{q,0} + \frac{1}{(n-1)!} A^K_{q,1} + \frac{1}{(n-2)!} A^K_{q,2} + \cdots + A^K_{q,n-1} \right)$$

(A 3.2)

for n = 0 we find

$$A^K_{q,0} = \frac{1}{\sqrt{q!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} \qquad \text{(A 3.3)}$$

the n = 1 coefficient turns out:

$$A^K_{q,1} = -\sqrt{\frac{1}{(q+1)!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J+1 & q & J-(q+1) \end{pmatrix}$$
$$- \sqrt{\frac{1}{q!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix}$$

$$A_{q,1}^{K} = -A_{q,0}^{K}\left\{1+\frac{1}{\sqrt{q+1}}\frac{\begin{pmatrix} J & K & J \\ J-1 & q & J-(q+1)\end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}}\right\} \qquad \text{(A 3.4)}$$

the n = 2 coefficient shall finally be calculated:

$$A_{q,2}^{K} = \sqrt{\frac{1}{2!\,(q+2)!}}\ \langle J\|\tilde{O}_K\|J\rangle \begin{pmatrix} J & K & J \\ -J+2 & q & J-(q+2)\end{pmatrix}$$

$$-\frac{1}{2\sqrt{q!}}\langle J\|\hat{O}_K\|J\rangle \begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}$$

$$+\frac{1}{\sqrt{q!}}\langle J\|\hat{O}_K\|J\rangle \begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}\left\{1+\frac{1}{\sqrt{q+1}}\frac{\begin{pmatrix} J & K & J \\ -J+1 & q & J-(q+1)\end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}}\right\}$$

$$A_{q,2}^{K} = A_{q,0}^{K}\,\frac{1}{2}\left\{1+\frac{2}{\sqrt{q+1}}\frac{\begin{pmatrix} J & K & J \\ -J+1 & q & J-(q+1)\end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}}+\frac{\sqrt{2}}{\sqrt{(q+1)(q+2)}}\frac{\begin{pmatrix} J & K & J \\ -J+2 & q & J-(q+2)\end{pmatrix}}{\begin{pmatrix} J & K & J \\ -J & q & J-q\end{pmatrix}}\right\}$$

(A 3.5)

As a starting point we calculate the coefficient

$$A_{0,0}^{K} = \langle J\|\tilde{O}_K\|J\rangle \begin{pmatrix} J & K & J \\ -J & 0 & J\end{pmatrix}$$

here

$$\langle J\|\hat{O}_K\|J\rangle = \frac{1}{2^K}\sqrt{\frac{(2J+K+1)!}{(2J-K)!}}$$

and from Edmonds[3)]

$$\begin{pmatrix} J & K & J \\ -J & 0 & J \end{pmatrix} = \begin{pmatrix} J & J & K \\ J & -J & 0 \end{pmatrix} = \frac{(2J)!}{\sqrt{(2J-K)!\,(2J+K+1)!}} \tag{A 3.6}$$

we find:

$$A^{K}_{0,0} = \frac{1}{2^K}\frac{(2J)!}{(2J-K)!} = S_K \tag{A 3.7}$$

From this the S_K-function is defined, namely

$$S_K = \frac{1}{2^K}\frac{(2J)!}{(2J-K)!} = J(J-1/2)(J-1)(J-3/2)\cdots\left(J-\frac{K-1}{2}\right) \tag{A 3.8}$$

Using the following recursion formula for 3j-symbols, Rothenberg[12)]

$$-\sqrt{(j_3+m_1+m_2+1)(j_3-m_1-m_2)}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3+1 \end{pmatrix} =$$

$$\sqrt{(j_1+m_1+1)(j_1-m_1)}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1+1 & m_2 & -m_3 \end{pmatrix} +$$

$$\sqrt{(j_2+m_2+1)(j_2-m_2)}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2+1 & -m_3 \end{pmatrix} \tag{A 3.9}$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}$$

$$j_1 = j_3 = J ; \quad j_2 = K$$

$$m_1 = J ; \quad m_2 = -q ; \quad m_3 = J - q + 1$$

$$-\sqrt{q(2J-q+1)} \begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} = \sqrt{(K-q+1)(K+q)} \begin{pmatrix} J & K & J \\ -J & q-1 & J-(q-1) \end{pmatrix}$$

$$\begin{pmatrix} J & K & J \\ -J & q & J-q \end{pmatrix} = -\sqrt{\frac{(K-q+1)(K+q)}{q(2J-q+1)}} \begin{pmatrix} J & K & J \\ -J & q & J-(q-1) \end{pmatrix} \qquad (3.10)$$

From this we find for the $A^K_{q,o}$ coefficient:

$$A^K_{q,0} = -\frac{1}{\sqrt{q!}} \langle J \| \tilde{O}_K \| J \rangle \sqrt{\frac{(K-q+1)(K+q)}{(2J-q+1)\, q}} \begin{pmatrix} J & K & J \\ -J & q-1 & J-(q-1) \end{pmatrix}$$

now

$$A^K_{q-1,0} = \frac{1}{\sqrt{(q-1)!}} \langle J \| \tilde{O}_K \| J \rangle \begin{pmatrix} J & K & J \\ -J & q-1 & J-(q-1) \end{pmatrix}$$

why

$$A^K_{q,0} = -\frac{1}{q} \sqrt{\frac{(K-q+1)(K+q)}{(2J-q+1)}}\, A^K_{q-1,0}$$

further we find

$$A^K_{q,0} = \frac{1}{q(q-1)} \sqrt{\frac{(K-q+1)(K-q+2)(K+q-1)(K+q)}{2^2\left(J-\frac{q-2}{2}\right)\left(J-\frac{q-1}{2}\right)}}\, A^K_{q-2,0}$$

$$\ldots$$

$$= (-1)^q \frac{1}{q!} \sqrt{\frac{(K-q+1)(K-q+2)\cdots(K+1)K\cdots(K+q-1)(K+q)}{2^q J\left(J-\frac{1}{2}\right)(J-1)\cdots\left(J-\frac{q-2}{2}\right)\left(J-\frac{q-1}{2}\right)}}\, A^K_{00}$$

on closed form

$$A^K_{q,0} = \frac{(-1)^q}{q!} \sqrt{\frac{(K+q)!}{2^q (K-q)!}}\; \frac{S_K}{\sqrt{S_q}} \qquad \text{(A 3.11)}$$

Now we want to calculate the coefficients $A^K_{q,1}$ and $A^K_{1,2}$ and to that end we again take the 3j-recursion formula from Rotenberg(A3. 9) and now put in:

$$j_1 = j_3 = J;\quad j_2 = K$$

$$m_1 = -J+n-1 \quad ;\; m_2 = q;\; m_3 = -J+n+q$$

$$-\sqrt{(n+q)(2J-n-q+1)} \begin{pmatrix} J & K & J \\ -J+n+1 & q & J-n-q+1 \end{pmatrix} =$$

$$\sqrt{n(2J-n+1)} \begin{pmatrix} J & K & J \\ -J+n & q & J-n-q \end{pmatrix}$$

$$+\sqrt{(K+q+1)(K-q)} \begin{pmatrix} J & K & J \\ -J+n-1 & q+1 & J-n-q \end{pmatrix}$$

(A3.1 2)

using

$$A^{K}_{q+1,0} = -\frac{1}{q+1}\sqrt{\frac{(K-q)(K+q+1)}{2\left(J-\frac{q}{2}\right)}}\;A^{K}_{q,0}$$

we find for $n \geq 1$

$$\begin{aligned}
A^{K}_{q,n} = &-\left[\frac{(K-q)(K+q+1)}{2(q+1)} + \sqrt{\left(J-\tfrac{n-1}{2}\right)\left(J-\tfrac{q}{2}\right)} - \sqrt{\left(J-\tfrac{n+q-1}{2}\right)\left(J-\tfrac{q}{2}\right)}\right]\times \\
&\qquad\times \frac{1}{n!}\,\frac{A^{K}_{q,0}}{\sqrt{\left(J-\frac{n-1}{2}\right)\left(J-\frac{q}{2}\right)}} \\
&+\frac{1}{n}\sqrt{\frac{(K-q)(K+q+1)}{2\left(J-\frac{n-1}{2}\right)}}\left[\frac{1}{(n-2)!}A^{K}_{q+1,1} + \frac{1}{(n-3)!}A^{K}_{q+1,2} + \cdots + A^{K}_{q+1,n-1}\right] \\
&+\frac{1}{n}\sqrt{\frac{\left(J-\frac{n+q-1}{2}\right)}{\left(J-\frac{n-1}{2}\right)}}\left[\frac{1}{(n-2)!}A^{K}_{q,1} + \frac{1}{(n-3)!}A^{K}_{q,2} + \cdots + A^{K}_{q,n-1}\right] \\
&-\left[\frac{1}{(n-1)!}A^{K}_{q,1} + \frac{1}{(n-2)!}A^{K}_{q,2} + \cdots + A^{K}_{q,n-1}\right]
\end{aligned}$$

(A3.13)

for <u>n = 1</u> we find the $A^{K}_{q,1}$ coefficient:

$$A^{K}_{q,1} = -A^{K}_{q,0}\sqrt{\frac{S_q}{S_1 S_{q+1}}}\left\{\frac{(K-q)(K+q+1)}{2(q+1)} + \sqrt{\frac{S_1 S_{q+1}}{S_q}} - \frac{S_{q+1}}{S_q}\right\}$$

(A3.14)

For n = 2 we find the $A^{K}_{1,2}$ coefficient

$$A^{K}_{1,2} = - A^{K}_{1,0}\left\{\frac{(K-1)(K+2)}{4}\left[\frac{(K-2)(K+3)}{12}\,\frac{S_1}{S_2} + \frac{1}{\sqrt{S_2}}\left(1-\frac{\sqrt{S_1 S_2}}{S_2}\right)\right] + \frac{1}{2}\left(1+\sqrt{\frac{S_2}{S_1 S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right\} \tag{A3.15}$$

APPENDIX 4

Diagonalization of the One Sublattice Hamiltonian

The diagonalization of a Hamiltonian bilinear in Fourier transformed Bose operators might be carried out by the Bogoliubov equation-of-motion-method. Here an equivalent method by Kowalska and Lindgård[26] based upon the theory of matrix calculus are used. The one sublattice Hamiltonian from (4.40) is

$$\mathcal{H} = \frac{1}{2}\sum_{q}\left(A_q a_q^+ a_q + A_{-q} a_{-q} a_{-q}^+ + B_q a_q a_{-q} + B_q^* a_q^+ a_{-q}^+\right) \tag{A4.1}$$

Written on matrix form we find an equivalent expression of the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\left\{a_q^+ a_{-q}\right\}\begin{Bmatrix} A_q & B_q^* \\ B_q & A_{-q}\end{Bmatrix}\begin{Bmatrix} a_q \\ a_{-q}^+\end{Bmatrix} = \frac{1}{2}\underline{X}^+\underline{\underline{\mathcal{H}}}\,\underline{X} \tag{A4.2}$$

where

$$\underline{X} = \begin{Bmatrix} a_q \\ a^+_{-q} \end{Bmatrix} \quad \text{and} \quad \underline{\underline{\mathcal{H}}} = \begin{Bmatrix} A_q & B^*_q \\ B_q & A_{-q} \end{Bmatrix}$$

Now we define the transformation

$$\begin{aligned} a_q &= \alpha_1 F_q + \alpha_2 F^+_{-q} \\ a_{-q} &= \beta_1 F_{-q} + \beta_2 F^+_q \end{aligned} \iff \begin{Bmatrix} a_q \\ a^+_{-q} \end{Bmatrix} = \begin{Bmatrix} \alpha_1 & \alpha_2 \\ \beta^*_2 & \beta^*_1 \end{Bmatrix} \begin{Bmatrix} F_q \\ F^+_{-q} \end{Bmatrix} = \underline{\underline{T}}\,\underline{Y}$$

(A4.3)

$$\underline{Y} = \begin{Bmatrix} F_q \\ F^+_{-q} \end{Bmatrix} \qquad \underline{\underline{T}} = \begin{Bmatrix} \alpha_1 & \alpha_2 \\ \beta^*_2 & \beta^*_1 \end{Bmatrix}$$

The opposite transformation is

$$\begin{aligned} F_q &= \alpha^*_1 a_q - \beta_2 a^+_{-q} \\ F_{-q} &= -\alpha_2 a^+_q + \beta^*_1 a_{-q} \end{aligned} \iff \begin{Bmatrix} F_q \\ F^+_{-q} \end{Bmatrix} = \begin{Bmatrix} \alpha^*_1 & -\beta_2 \\ -\alpha^*_2 & \beta_1 \end{Bmatrix} \begin{Bmatrix} a_q \\ a^+_{-q} \end{Bmatrix} = \underline{\underline{T}}^{-1} \underline{X}$$

(A4.4)

$$\underline{\underline{T}}^{-1} = \begin{Bmatrix} \alpha^*_1 & -\beta_2 \\ -\alpha^*_2 & \beta_1 \end{Bmatrix}$$

The fact that a_q and a^+_q obey the Bose commution relations, (BCR) gives the following relations of the transformation constants α_1, α_2, β_1 and β_2

$$[a_q, a_q^+] = [(\alpha_1 F_q + \alpha_2 F_{-q}^+), (\alpha_1^* F_{-q}^+ + \alpha_2^* F_{-q})] = |\alpha_1|^2 - |\alpha_2|^2 = 1$$

$$[a_{-q}, a_{-q}^+] = [(\beta_1 F_q + \beta_2 F_q^+), (\beta_1^* F_{-q}^+ + \beta_2^* F_q)] = |\beta_1|^2 - |\beta_2|^2 = 1$$

$$[a_q, a_{-q}] = [(\alpha_1 F_q + \alpha_2 F_{-q}^+), (\beta_1 F_{-q} + \beta_2 F_q^+)] = \alpha_1\beta_2 - \alpha_2\beta_1 = 0$$

(A4.5)

The transformation matrix $\underline{\underline{T}}$ fulfill according to the Bose commutator relations the relation

$$\underline{\underline{T}} \cdot \underline{\underline{T}}^{-1} = \begin{Bmatrix} \alpha_1 & \alpha_2 \\ \beta_2^* & \beta_1^* \end{Bmatrix} \begin{Bmatrix} \alpha_1^* & -\beta_2 \\ -\alpha_2^* & \beta_1 \end{Bmatrix} = \begin{Bmatrix} (|\alpha_1|^2 - |\alpha_2|^2) & -(\alpha_1\beta_2 - \alpha_2\beta_1) \\ \alpha_1^*\beta_2^* - \alpha_2^*\beta_1^* & (|\beta_1|^2 - |\beta_2|^2) \end{Bmatrix} = \begin{Bmatrix} 1 & 0 \\ 0 & 1 \end{Bmatrix}$$

Because of the Bose commutator relations the transformation that diagonalizes the Hermitian Hamiltonian is non-unitar. To show this we calculate $\underline{\underline{T}}^+$ and see that it is different from $\underline{\underline{T}}^{-1}$

$$\underline{\underline{T}}^+ = \begin{Bmatrix} \alpha_1^* & \beta_2 \\ \alpha_2^* & \beta_1 \end{Bmatrix} \neq \underline{\underline{T}}^{-1} \qquad \text{(A4.6)}$$

<u>The eigenvalues of the Hamiltonian</u>

$$\mathcal{H} = \tfrac{1}{2}\, \underline{X}^+ \underline{\underline{\mathcal{H}}}\, \underline{X} = \tfrac{1}{2} (\underline{\underline{T}}^{-1} \underline{X})^+ \underline{\underline{T}}^+ \underline{\underline{\mathcal{H}}}\, \underline{\underline{T}} (\underline{\underline{T}}^{-1} \underline{X}) = \tfrac{1}{2}\, \underline{Y}^+ \underline{\underline{E}}\, \underline{Y}$$

(A4.7)

$\underline{\underline{E}} = \underline{\underline{T}}^{\dagger} \underline{\underline{\ell}}\, \underline{\underline{T}}$ is diagonal

$\underline{Y} = \underline{\underline{T}}^{-1} \underline{X}$ and the opposite $\underline{X} = \underline{\underline{T}}\, \underline{Y}$

Written out we have

$$\begin{Bmatrix} A_q & B_q^* \\ B_q & A_{-q} \end{Bmatrix} \begin{Bmatrix} \alpha_1 & \alpha_2 \\ \beta_2^* & \beta_1^* \end{Bmatrix} = \begin{Bmatrix} E_q & 0 \\ 0 & E_{-q} \end{Bmatrix} \begin{Bmatrix} \alpha_1 & -\alpha_2 \\ -\beta_2^* & \beta_1^* \end{Bmatrix} \qquad \text{(A4. 8)}$$

We introduce a matrix $\underline{\underline{B}}$ and have for the two coloum vectors $\underline{u}_1$, $\underline{u}_2$:

$$\underline{\underline{B}} = \begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix} \; ; \quad \underline{u}_1 = \begin{Bmatrix} \alpha_1 \\ \beta_2^* \end{Bmatrix} \; ; \quad \underline{u}_2 = \begin{Bmatrix} \alpha_2 \\ \beta_1^* \end{Bmatrix}$$

$$\begin{Bmatrix} A_q & B_q^* \\ B_q & A_{-q} \end{Bmatrix} \begin{Bmatrix} \alpha_1 \\ \beta_2^* \end{Bmatrix} = E_q \begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix} \begin{Bmatrix} \alpha_1 \\ -\beta_2^* \end{Bmatrix} = E_q \begin{Bmatrix} \alpha_1 \\ \beta_2^* \end{Bmatrix}$$

$$\begin{Bmatrix} A_q & B_q^* \\ B_q & A_{-q} \end{Bmatrix} \begin{Bmatrix} \alpha_2 \\ \beta_1^* \end{Bmatrix} = -E_{-q} \begin{Bmatrix} 1 & 0 \\ 0 & -1 \end{Bmatrix} \begin{Bmatrix} -\alpha_2 \\ \beta_1^* \end{Bmatrix} = E_{-q} \begin{Bmatrix} \alpha_2 \\ \beta_1^* \end{Bmatrix}$$

which gives the following eigenvalue determinant equation

$$\begin{vmatrix} A_q - \lambda & B_q^* \\ B_q & A_{-q} + \lambda \end{vmatrix} = 0$$

$$-\lambda^2 + \lambda \left(A_q - A_{-q} \right) + A_q A_{-q} - |B_q|^2 = 0$$

The energy is an even function of q, as it is impossible to see any difference in the +q and -q directions.

$$\Rightarrow A_q = A_{-q}$$

$$\lambda^2 - (A_q^2 - |B_q|^2) = 0$$

$$\lambda = \pm\sqrt{A_q^2 - |B_q|^2} = E_{\pm q} \tag{A4.9}$$

The eigen vectors belonging to the eigenvalue E_{+q} (B_q real)

$$\begin{aligned}
\alpha_1 &= \left\{ \frac{1}{2} + \frac{1}{2}\frac{A_q}{\sqrt{A_q^2 - |B_q|^2}} \right\}^{1/2} \\
\alpha_2 &= -\left\{ -\frac{1}{2} + \frac{1}{2}\frac{A_q}{\sqrt{A_q^2 - |B_q|^2}} \right\}^{1/2} \\
\beta_1 &= \left\{ \frac{1}{2} + \frac{1}{2}\frac{A_q}{\sqrt{A_q^2 - |B_q|^2}} \right\}^{1/2} \\
\beta_2 &= -\left\{ -\frac{1}{2} + \frac{1}{2}\frac{A_q}{\sqrt{A_q^2 - |B_q|^2}} \right\}^{1/2}
\end{aligned} \tag{A4.10}$$

The "old" Bose operators in the diagonal representation:

$$\begin{aligned}
a_q^+ a_q &= (\alpha_1^* F_q^+ + \alpha_2^* F_{-q})(\alpha_1 F_q + \alpha_2 F_{-q}^+) \\
&= \left(\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_q^+ F_q + \left(-\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_{-q}^+ F_{-q} \\
&\quad + \left(-\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) - \frac{B_q}{2E_q}\left(F_q^+ F_{-q}^+ + F_q F_{-q}\right)
\end{aligned} \tag{A4.11}$$

$$a_q a_{-q} = (\alpha_1 F_q + \alpha_2 F_{-q}^{+})(\beta_1 F_{-q} + \beta_2 F_q^{+})$$

$$= -\frac{B_q}{2E_q}(F_q^{+}F_q + F_{-q}^{+}F_{-q} + 1)$$

$$+ \left(\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_q F_{-q} + \left(-\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_q^{+} F_{-q}^{+} \qquad \text{(A4.12)}$$

$$a_q^{+} a_{-q}^{+} = (\alpha_1^{*} F_q^{+} + \alpha_2^{*} F_{-q})(\beta_1^{*} F_{-q}^{+} + \beta_2^{*} F_q)$$

$$= -\frac{B_q}{2E_q}(F_q^{+}F_q + F_{-q}^{+}F_{-q} + 1)$$

$$+ \left(-\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_q F_{-q} + \left(\frac{1}{2} + \frac{1}{2}\frac{A_q}{E_q}\right) F_q^{+} F_{-q}^{+} \qquad \text{(A4.13)}$$

<u>The Hamiltonian expressed in the "new" Bose operators:</u>

$$\mathcal{H} = \sum_q \frac{1}{2} A_q (a_q^{+} a_q + a_q a_{-q}^{+}) + \frac{1}{2}(B_q a_q a_{-q} + B_q^{*} a_q^{+} a_{-q}^{+})$$

$$= \sum_q \left(\frac{1}{2} \frac{A_q^2 - |B_q|^2}{E_q} F_q^{+} F_q + \frac{1}{2} \frac{A_q^2 - |B_q|^2}{E_q} F_{-q}^{+} F_{-q} + \frac{1}{2} \frac{A_q^2 - |B_q|^2}{E_q} \right)$$

$$= \sum_q \sqrt{A_q^2 - |B_q|^2} \, (F_q^{+} F_q + \tfrac{1}{2})$$

$$= \sum_q E_q (\hat{n}_q + \tfrac{1}{2}) \qquad \text{(A4.14)}$$

$$E_q = \sqrt{A_q^2 - |B_q|^2}$$
$$\hat{n}_q = F_q^+ F_q \tag{A4.15}$$

in which way the Hamiltonian has been brought to the well-known "oscillator-form". A similar expression can be obtained with the other eigenvalue.

Some selected matrix elements:

$$\langle n_q | a_q^+ a_q | n_q \rangle = \frac{A_q}{E_q}(n_q + \tfrac{1}{2}) - \tfrac{1}{2} \tag{A4.16}$$

$$\langle n_q | a_q a_{-q} | n_q \rangle = -\frac{B_q}{E_q}(n_q + \tfrac{1}{2}) \tag{A4.17}$$

$$\langle n_q | a_q^+ a_{-q}^+ | n_q \rangle = -\frac{B_q}{E_q}(n_q + \tfrac{1}{2}) \tag{A4.18}$$

APPENDIX 5

The Spinwave Dispersion Constants of a Hexagonal Bravais Lattice in the c-axis Representation

With the intention of doing an explicit calculation of the temperature dependence of the magneto crystalline anisotropy, the interactions of the magnetic Bravais lattice is specified. We include in the Hamiltonian an isotop exchange interaction, single-ion magneto crystalline anisotropy, single-ion magnetostriction and the effect of an external, applied magnetic field. Then in an interacting magnon-magnon calculation we compute the contribution from the different parts of the Hamiltonian to the magnon dispersion constants

Isotop exchange of a Bravais lattice

An intra lattice isotrop exchange interaction might be described by

$$\mathcal{H}_{ex} = -\sum_{l>l'} \mathcal{J}(\bar{R}_{ll'})\, \underline{J}_l \cdot \underline{J}_{l'} \tag{A5.1}$$

here l and l' mean lattice sites of the magnetic crystal, $\underline{J}_l$ and $\underline{J}_{l'}$ the total spins of the respective lattice sites and the exchange function $\mathcal{J}(R_{ll'})$ depends on the lattice distance $R_{ll'} = R_l - R_{l'}$. Doing a Bose operator expansion of the spins we find for $\mathcal{H}_{ex}$, table 1

$$\begin{aligned}\mathcal{H}_{ex} = -\tfrac{1}{2} N S_1^2 \mathcal{J}(0) + \sum_{l>l'} \mathcal{J}(\bar{R}_{ll'}) \Big\{ & S_1 [a_l^+ a_l + a_{l'}^+ a_{l'} - a_l^+ a_{l'} - a_l a_{l'}^+] \\ & + (S_1 - \sqrt{S_2}) [a_l^+ a_{l'}^+ a_{l'} a_{l'} + a_l^+ a_l^+ a_l a_{l'} \\ & \quad + a_l a_{l'}^+ a_{l'}^+ a_{l'} + a_l^+ a_l a_l a_{l'}^+] \\ & - a_l^+ a_l a_{l'}^+ a_{l'} \Big\}\end{aligned} \tag{A5.2}$$

Making a fourier transformation, following table 8, we find for the non-interacting part:

$$(\mathcal{H}_{ex})_0 = -\tfrac{1}{2} N \mathcal{J}(0) J(J+1) + \sum_k \tfrac{1}{2} S_1 (\mathcal{J}(0) - \mathcal{J}(\underline{k}))(a_k^+ a_k + a_k a_k^+) \tag{A5.3}$$

giving the contributions to the dispersion constants

$$E_0(ex) = -\tfrac{1}{2} N \mathcal{J}(0) J(J+1) \tag{A5.4}$$

$$A_k(ex) = S_1 (\mathcal{J}(0) - \mathcal{J}(\underline{k})) \tag{A5.5}$$

The interacting part of the exchange Hamiltonian becomes,

$$(\mathcal{H}_{ex})_1 = \frac{1}{2N}\sum_{\substack{K_1K_2\\K_3K_4}}\left\{2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_4)+\mathcal{J}(\underline{K}_1)\right)-\mathcal{J}(\underline{K}_4-\underline{K}_2)\right\}\times$$
$$\times\,\delta_{K_1+K_2,\,K_3+K_4}\; a^{+}_{K_1}a^{+}_{K_2}a_{K_3}a_{K_4}$$

(A5.6)

By use of table 9 we do a Hartree-Fock decoupling of the interacting part of the exchange Hamiltonian and we find for the contributions to the dispersion constants:

$$\Delta E_0(ex) = \frac{1}{2N}\sum_{K_1K_2}\left\{\mathcal{J}(0)-\mathcal{J}(\underline{K}_1+\underline{K}_2)-2(S_1-\sqrt{S_2})\left(3\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right)\right\}\times$$
$$\times\langle a^{+}_{K_1}a_{K_1}\rangle\langle a^{+}_{K_2}a_{K_2}\rangle$$
$$-\frac{1}{2N}\sum_{K_1K_2}\left\{2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right)-\mathcal{J}(\underline{K}_1-\underline{K}_2)\right\}\times$$
$$\times\langle a^{+}_{K_1}a^{+}_{-K_1}\rangle\langle a_{K_2}a_{K_2}\rangle$$
$$+\frac{1}{2N}\sum_{K_1}\left\{\mathcal{J}(0)+\mathcal{J}(\underline{K}_1-\underline{K}_2)-4(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\right)\right\}\langle a^{+}_{K_1}a_{K_1}\rangle$$

(A5.7)

$$\Delta A_K(ex) = \frac{1}{N}\sum_{K_1}\left\{4(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K})+\mathcal{J}(\underline{K}_1)\right)-\mathcal{J}(0)-\mathcal{J}(\underline{K}-\underline{K}_1)\right\}\langle a^{+}_{K_1}a_{K_1}\rangle$$

(A5.8)

$$\Delta B_K(ex) = \frac{1}{N}\sum_{K_1}\left\{2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K})\right)-\mathcal{J}(\underline{K}_1-\underline{K})\right\}\langle a^{+}_{K_1}a^{+}_{K_1}\rangle$$

(A5.9)

$$\Delta B^{*}_K(ex) = \frac{1}{N}\sum_{K_1}\left\{2(S_1-\sqrt{S_2})\left(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K})\right)-\mathcal{J}(\underline{K}_1-\underline{K})\right\}\langle a_{K_1}a_{K_1}\rangle$$

(A5.10)

Magneto Crystalline Anisotropy

In a c-axis representation the single-ion anisotropy of a hexagonal lattice is

$$\mathcal{H}_{an} = \sum_i \left\{ B_2^0 O_2^0(c) + B_4^0 O_4^0(c) + B_6^0 O_6^0(c) + B_6^6 O_6^6(c) \right\}_i \qquad \text{(A5.11)}$$

B_K^q being the crystal field parameters and $O_K^q(c)$ the Stevens operators. Doing a Bose operator expansion of the single-ion anisotropy we find, table 5

$$\begin{aligned}\mathcal{H}_{an} = {} & N\left(2S_2B_2^0 + 8S_4B_4^0 + 16S_6B_6^0\right) \\ & - \frac{1}{S_1}\left(6S_2B_2^0 + 80S_4B_4^0 + 336S_6B_6^0\right)\sum_l a_l^+ a_l \\ & + \frac{1}{2S_2}\left(6S_2B_2^0 + 360S_4B_4^0 + 3360S_6B_6^0\right)\sum_l a_l^+ a_l^+ a_l a_l\end{aligned}$$

(A5.12)

Making a Fourier transformation of the Hamiltonian we find for the non-interacting part of the anisotropy Hamiltonian, table 8

$$\begin{aligned}(\mathcal{H}_{an})_0 = {} & N\left(B_2^0 2S_2\left(1+\frac{3}{2S_1}\right) + B_4^0 8S_4\left(1+\frac{5}{S_1}\right) + B_6^0 16S_6\left(1+\frac{21}{2S_1}\right)\right) \\ & - \frac{1}{S_1}\left(6S_2B_2^0 + 80S_4B_4^0 + 336S_6B_6^0\right)\sum_k \frac{1}{2}\left(a_k^+ a_k + a_k a_k^+\right)\end{aligned}$$

(A5.13)

giving the following contributions to the dispersion constants

$$E_0(an) = N\left(2S_2 B_2^0\left(1+\frac{3}{2S_1}\right)+8S_4 B_4^0\left(1+\frac{5}{S_1}\right)+16S_6 B_6^0\left(1+\frac{21}{2S_2}\right)\right) \quad \text{(A5.14)}$$

$$A_K(an) = -\frac{1}{S_1}\left(6S_2 B_2^0+80S_4 B_4^0+336S_6 B_6^0\right) \quad \text{(A5.15)}$$

The interacting part of single-ion anisotropy Hamiltonian becomes, table 8

$$(\mathcal{H}_{an})_1 = \frac{1}{2S_2}\left(6S_2 B_2^0+360S_4 B_4^0+3360 S_6 B_6^0\right) \times$$
$$\times \frac{1}{N}\sum_{\substack{K_1K_2\\K_3K_4}} \delta_{K_1+K_2,K_3+K_4}\, a_{K_1}^{\dagger} a_{K_2}^{\dagger} a_{K_3} a_{K_4} \quad \text{(A5.16)}$$

from where we, through a Hartree-Fock decoupling, find the contributions to the dispersion constants, table 9:

$$\Delta E_0(an) = -\frac{1}{2S_2}\left(6S_2 B_2^0+360S_4 B_4^0+3360 S_6 B_6^0\right)\times\Big[2\sum_K \langle a_K^{\dagger} a_K\rangle$$
$$+\frac{1}{N}\sum_{K_1K_2}\big(2\langle a_{K_1}^{\dagger} a_{K_1}\rangle\langle a_{K_2}^{\dagger} a_{K_2}\rangle+\langle a_{K_1}^{\dagger} a_{-K_1}^{\dagger}\rangle\langle a_{K_2} a \ldots \quad \text{(A5.17)}$$

$$\Delta A_K(an) = \frac{1}{2S_2}\left(6S_2 B_2^0+360S_4 B_4^0+3360 S_6 B_6^0\right)\frac{4}{N}\sum_{K_1}\langle a_{K_1}^{\dagger} a_{K_1}\rangle \quad \text{(A5.18)}$$

$$\Delta B_K(an) = \frac{1}{2S_2}\left(6S_2 B_2^0+360S_4 B_4^0+3360 S_6 B_6^0\right)\frac{2}{N}\sum_{K_1}\langle a_{K_1}^{\dagger} a_{-K_1}^{\dagger}\rangle \quad \text{(A5.19)}$$

$$\Delta B_K^{*}(an) = \frac{1}{2S_2}\left(6S_2 B_2^0+360S_4 B_4^0+3360 S_6 B_6^0\right)\frac{2}{N}\sum_{K_1}\langle a_{K_1} a_{-K_1}\rangle \quad \text{(A5.20)}$$

Magnetostriction

In a c-axis representation the single-ion magnetostriction of a hexagonal lattice is:

$$
\begin{aligned}
\mathcal{H}_{me} = -\sum_{l} \Big\{ & \left(B_{20}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) O_2^0(c) + \left(B_{40}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) O_4^0(c) \\
& + \left(B_{60}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) O_6^0(c) + \left(B_{66}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) O_6^6(c) \\
& + B_{22}^{\gamma}\left(\bar{\epsilon}_1^{\gamma} O_2^2(c) + \bar{\epsilon}_2^{\gamma} O_2^2(s)\right) + B_{42}^{\gamma}\left(\bar{\epsilon}_1^{\gamma} O_4^2(c) + \bar{\epsilon}_2^{\gamma} O_4^2(s)\right) \\
& + B_{62}^{\gamma}\left(\bar{\epsilon}_1^{\gamma} O_6^2(c) + \bar{\epsilon}_2^{\gamma} O_6^2(s)\right) + B_{44}^{\gamma}\left(\bar{\epsilon}_1^{\gamma} O_4^4(c) + \bar{\epsilon}_2^{\gamma} O_4^4(s)\right) \\
& + B_{64}^{\gamma}\left(\bar{\epsilon}_1^{\gamma} O_6^4(c) + \bar{\epsilon}_2^{\gamma} O_6^4(s)\right) + B_{21}^{\epsilon}\left(\bar{\epsilon}_1^{\epsilon} O_2^1(c) + \bar{\epsilon}_2^{\epsilon} O_2^1(s)\right) \\
& + B_{41}^{\epsilon}\left(\bar{\epsilon}_1^{\epsilon} O_4^1(c) + \bar{\epsilon}_2^{\epsilon} O_4^1(s)\right) + B_{61}^{\epsilon}\left(\bar{\epsilon}_1^{\epsilon} O_6^1(c) + \bar{\epsilon}_2^{\epsilon} O_6^1(s)\right) \\
& + B_{65}^{\epsilon}\left(\bar{\epsilon}_1^{\epsilon} O_6^5(c) + \bar{\epsilon}_2^{\epsilon} O_6^5(s)\right) \Big\}_l
\end{aligned}
\qquad \text{(A5.21)}
$$

In the further transformation to Bose operators only even-valued c-Stevens operators are included, as odd-valued Stevens operators do not contribute in a temperature calculation. In this way the ϵ_2^{γ} , ϵ_1^{ϵ} , and ϵ_2^{ϵ} strains are excluded from the further calculations.

$$
\begin{aligned}
\mathcal{H}_{me} = -N\Big(& 2S_2\left(B_{20}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) + 8S_4\left(B_{40}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) \\
& + 16S_6\left(B_{60}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right)\Big) \\
& + \frac{1}{S_1}\Big(6S_2\left(B_{20}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) + 80S_4\left(B_{40}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right) \\
& + 336S_6\left(B_{60}^{\alpha,1}\bar{\epsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\epsilon}^{\alpha,2}\right)\Big)\sum_{l} a_l^{+} a_l
\end{aligned}
$$

$$-\left(B_{22}^{\gamma}\bar{\varepsilon}_1^{\gamma}\sqrt{S_2} + B_{42}^{\gamma}\bar{\varepsilon}_1^{\gamma}\frac{6S_4}{\sqrt{S_2}} + B_{62}^{\gamma}\bar{\varepsilon}_1^{\gamma}\frac{16S_6}{\sqrt{S_2}}\right)\sum_l \left(a_l^+a_l^+ + a_la_l\right)$$

$$-\frac{1}{2S_2}\Big(6S_2\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)+360S_4\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+3360S_6\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\Big)\sum_l a_l^+a_l^+a_la_l$$

$$+\Big(B_{22}^{\gamma}\bar{\varepsilon}_1^{\gamma}\sqrt{S_2}\sqrt{\frac{S_2}{S_1S_3}}\left(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)+B_{42}^{\gamma}\bar{\varepsilon}_1^{\gamma}\frac{6S_4}{\sqrt{S_2}}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)$$

$$+B_{62}^{\gamma}\bar{\varepsilon}_1^{\gamma}\frac{16S_6}{\sqrt{S_2}}\sqrt{\frac{S_2}{S_1S_3}}\left(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)\Big)\sum_l\left(a_l^+a_l^+a_l^+a_l+a_l^+a_la_la_l\right)$$

$$-\left(B_{44}^{\gamma}\bar{\varepsilon}_1^{\gamma}2\sqrt{S_4}+B_{64}^{\gamma}\bar{\varepsilon}_1^{\gamma}\frac{20S_6}{\sqrt{S_4}}\right)\sum_l\left(a_l^+a_l^+a_l^+a_l^+ + a_la_la_la_l\right)$$

(A5. 22)

Making a Fourier transformation and a Hartree-Fock decouling we find the contributions from the magnetostriction to the dispersion constants, namely

$$E_0(me) = -N\Big\{2S_2\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\left(1+\frac{3}{2S_1}\right)$$

$$+8S_4\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\left(1+\frac{5}{S_1}\right)$$

$$+16S_6\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\left(1+\frac{21}{2S_1}\right)\Big\} \qquad \text{(A5. 23)}$$

$$A_K(me) = \frac{1}{S_1}\Big\{6S_2\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)+80S_4\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)$$

$$+360\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)S_6\Big\} \qquad \text{(A5. 24)}$$

$$B_K(me) = -\left(B_{22}^{r}\bar{\varepsilon}_1^{r}\sqrt{S_2} + B_{42}^{r}\bar{\varepsilon}_1^{r}\frac{6S_4}{\sqrt{S_2}} + B_{62}^{r}\bar{\varepsilon}_1^{r}\frac{16S_6}{\sqrt{S_2}} \right) \qquad \text{(A5. 25)}$$

$$\begin{aligned}
\Delta E_0(me) = {} & \frac{1}{S_2}\Big[6S_2\left(B_{20}^{\alpha_1 1}\bar{\varepsilon}^{\alpha_1 1} + B_{20}^{\alpha_1 2}\bar{\varepsilon}^{\alpha_1 2}\right) + 360S_4\left(B_{40}^{\alpha_1 1}\bar{\varepsilon}^{\alpha_1 1} + B_{40}^{\alpha_1 2}\bar{\varepsilon}^{\alpha_1 2}\right) \\
& + 3360S_6\left(B_{60}^{\alpha_1 1}\bar{\varepsilon}^{\alpha_1 1} + B_{60}^{\alpha_1 2}\bar{\varepsilon}^{\alpha_1 2}\right)\Big] \times \Big\{ 2\sum_K \langle a_K^+ a_K\rangle \\
& + \frac{1}{N}\sum_{K_1K_2}\left(2\langle a_{K_1}^+ a_{K_1}\rangle\langle a_{K_2}^+ a_{K_2}\rangle + \langle a_{K_1}^+ a_{K_1}^+\rangle\langle a_{K_2} a_{K_2}\rangle\right)\Big\} \\
& - \Big\{ B_{22}^{r}\bar{\varepsilon}_1^{r}\sqrt{S_2}\sqrt{\frac{S_2}{S_1S_3}}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) + B_{42}^{r}\bar{\varepsilon}_1^{r}\frac{6S_4}{\sqrt{S_2}}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{3}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) \\
& + B_{62}^{r}\bar{\varepsilon}_1^{r}\frac{40S_6}{\sqrt{S_2}}\sqrt{\frac{S_2}{S_1S_3}}\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\Big\} \Big\{ \frac{3}{2}\sum_{K_1}\left(\langle a_{K_1}^+ a_{-K_1}^+\rangle + \langle a_{K_1} a_{-K_1}\rangle\right) \\
& + \frac{3}{N}\sum_{K_1K_2}\langle a_{K_1}^+ a_{K_1}\rangle\left(\langle a_{K_2}^+ a_{-K_2}^+\rangle + \langle a_{K_2} a_{K_2}\rangle\right)\Big\} \\
& + \Big\{ B_{44}^{r}\bar{\varepsilon}_1^{r}2\sqrt{S_4} + B_{64}^{r}\bar{\varepsilon}_1^{r}\frac{20S_6}{\sqrt{S_4}}\Big\}\frac{3}{N}\sum_{K_1K_2}\Big(\langle a_{K_1}^+ a_{-K_1}^+\rangle\langle a_{K_2}^+ a_{-K_2}^+\rangle \\
& + \langle a_{K_1} a_{K_1}\rangle\langle a_{K_2} a_{K_2}\rangle\Big)
\end{aligned}$$

(A5. 26)

$$\begin{aligned}
\Delta A_K(me) = {} & \mathcal{K}(a^+a^+aa)\frac{4}{N}\sum_K\langle a_K^+ a_K\rangle + \\
& \mathcal{K}(a^+a^+a^+a + a^+aaa)\frac{3}{N}\sum_K\left(\langle a_K^+ a_{-K}^+\rangle + \langle a_K a_K\rangle\right)
\end{aligned}$$

(A 5. 27)

$$\begin{aligned}
\Delta B_K(me) = {} & \mathcal{K}(a^+a^+aa)\frac{2}{N}\sum_K\langle a_K^+ a_{-K}^+\rangle \\
& + \mathcal{K}(a^+a^+a^+a + a^+aaa)\frac{6}{N}\sum_K\langle a_K^+ a_K\rangle \\
& + \mathcal{K}(a^+a^+a^+a^+ + aaaa)\frac{12}{N}\sum_K\langle a_K a_K\rangle \qquad \text{(A5. 28)}
\end{aligned}$$

Applied Magnetic Field

A magnetic field applied in the c-direction gives the following Zeeman-contribution to the Hamiltonian of the hexagonal Bravais lattice

$$\begin{aligned}\mathcal{H}_{Zee} &= -g\mu_B H \sum_{\ell} J_{\ell}^{z} \\ &= -g\mu_B H J N - g\mu_B H \sum_{\ell} a_{\ell}^{+} a_{\ell} \\ &= -g\mu_B H N (J-\tfrac{1}{2}) - g\mu_B H \sum_{\ell} \tfrac{1}{2} (a_{\ell}^{+} a_{\ell} + a_{\ell} a_{\ell}^{+})\end{aligned} \tag{A5.29}$$

Doing a Fourier transformation we find the contributions to the dispersion-constants

$$E_0(Zee) = -g\mu_B H N (J-\tfrac{1}{2}) \tag{A5.30}$$

$$A_K(Zee) = -g\mu_B H \tag{A5.31}$$

APPENDIX 6

A Model Calculation of the Characteristic Functions $\Delta M(T)$ and $b(T)$

The temperature dependence of the Stevens operators has been expressed through the two characteristic functions $\Delta M(T)$ and $b(T)$. $\Delta M(T)$ is connected with the relative magnetization and $b(T)$ takes into account the noncircular spin precession about the direction of magnetization. They are according to (4.55) and appendix 4 given by

$$\Delta M(T) = \frac{1}{S_1 N} \sum_{q} \langle a_q^{+} a_q \rangle = \frac{1}{S_1 N} \sum_{q} \left\{ \frac{A_q}{\varepsilon_q} (\langle n_q \rangle + \tfrac{1}{2}) - \tfrac{1}{2} \right\} \tag{A6.1}$$

$$b(T) = \frac{1}{S_1 N} \sum_q \langle a_{-q} a_q \rangle = -\frac{1}{S_1 N} \sum_q \frac{B_q}{E_q} \left(\langle n_q \rangle + \frac{1}{2} \right) \qquad \text{(A6.2)}$$

Here $\langle n_q \rangle$ is the Bose factor, E_q the energy, A_q and B_q the dispersion relation constants.
The energy is

$$E_q = \sqrt{A_q^2 - B_q^2} \qquad \text{(A6.3)}$$

We are now going to set up a model calculation of the two characteristic functions $\Delta M(T)$ and $b(T)$ taking into account the fact that the dispersion relations are not equal in different high symmetry directions in the q-space. We calculate $\Delta M(T)$ and $b(T)$ on the basis of two models, one with quadratic q-dependence of the dispersion relations in both the c-direction ($\parallel$ direction) and in the basal plane direction ($\perp$-direction) and another model with quadratic q-dependence of the dispersion relation in the c-direction and with linear q-dependence of the dispersion relation in the basal plane direction.

Model no. 1: Quadratic q-Dependence of the Dispersion Relations in both c-Direction and Basal Plane Direction

The two characteristic functions are

$$\Delta M(T) = \frac{1}{S_1 N} \sum_q \left\{ \frac{A_q}{E_q} \left(\langle n_q \rangle + \frac{1}{2} \right) - \frac{1}{2} \right\}$$

$$= \frac{V_c}{S_1 (2\pi)^3} \int_q \left\{ \frac{A_q}{E_q} \left(\langle n_q \rangle + \frac{1}{2} \right) - \frac{1}{2} \right\} d\bar{q} \qquad \text{(A6.4)}$$

$$b(T) = -\frac{1}{S_1 N} \sum_q \left\{ \frac{B_q}{E_q} \left(\langle n_q \rangle + \frac{1}{2} \right) \right\}$$

$$= -\frac{V_c}{S_1 (2\pi)^3} \int_q \frac{B_q}{E_q} \left(\langle n_q \rangle + \frac{1}{2} \right) d\bar{q} \qquad \text{(A6.5)}$$

We have used the standard transformation from summation to integration

$$\sum_{q} \rightarrow \frac{V}{(2\pi)^3} \int_{\bar{q}} d\bar{q} \tag{A6.6}$$

where $V = V_c N$ is the volume of the crystal, V_c the volume of a unit cell and N the number of unit cells. Further we have for the volume element

$$d\bar{q} = dq_x\, dq_y\, dq_z = q_\perp\, dq_\perp\, dq_\parallel\, d\varphi \tag{A6.7}$$

The dispersion relation constants are

$$\mathcal{A}_q = \alpha + \beta_\perp q_\perp^2 + \beta_\parallel q_\parallel^2 \tag{A6.8}$$

$$\mathcal{B}_q = \gamma \tag{A6.9}$$

and the energy

$$\mathcal{E}_q = \Delta + J_\perp q_\perp^2 + J_\parallel^{(2)} q_\parallel^2 + J_\parallel^{(1)} q_\parallel^4 \tag{6.10}$$

From (A6.3) and (A6.10) we find the connexions between the dispersion relation parameters $\alpha, \beta_\perp, \beta_\parallel$ and γ and the energy parameters Δ, $J_\perp, J_\parallel^{(1)}$ and $J_\parallel^{(2)}$.

From (A6.8) we have

$$\mathcal{A}_q^{\parallel} = \alpha + \beta_\parallel q_\parallel^2$$

$$\mathcal{B}_q = \gamma$$

and therefore from (A6.3)

$$(\mathcal{E}_q^{\parallel})^2 = (\mathcal{A}_q^{\parallel})^2 - \mathcal{B}_q^2 = \beta_\parallel^2 q_\parallel^4 + 2\alpha\beta_\parallel q_\parallel^2 + \alpha^2 - \gamma^2 \tag{A6.11}$$

From (A6.10) we find

$$\mathcal{E}_q^{\parallel} = J_{\parallel}^{(1)} q_{\parallel}^4 + J_{\parallel}^{(2)} q_{\parallel}^2 + \Delta \qquad \text{(A6.12)}$$

and therefore

$$(\mathcal{E}_q^{\parallel})^2 \cong \left[2 J_{\parallel}^{(1)} \Delta + (J_{\parallel}^{(2)})^2 \right] q_{\parallel}^4 + 2 J_{\parallel}^{(2)} \Delta q_{\parallel}^2 + \Delta^2$$

We therefore have the following relations for the parameters

$$\beta_{\parallel}^2 \cong (J_{\parallel}^{(2)})^2 + 2 J_{\parallel}^{(1)} \Delta \qquad \text{(A6.13)}$$

$$\alpha \beta_{\parallel} \cong J_{\parallel}^{(2)} \Delta \qquad \text{(A6.14)}$$

$$\Delta = \sqrt{\alpha^2 - \gamma^2} \qquad \text{(A6.15)}$$

For the basal plane direction we find from (A6.8)

$$\mathcal{A}_q^{\perp} = \alpha + \beta_{\perp} q_{\perp}^2$$

$$\mathcal{B}_q = \gamma$$

and therefore from (A6.3)

$$(\mathcal{E}_q^{\perp})^2 = (\mathcal{A}_q^{\perp})^2 - \mathcal{B}_q^2 \cong 2 \alpha \beta_{\perp} q_{\perp}^2 + \alpha^2 - \gamma^2 \qquad \text{(A6.16)}$$

From (A6.10) we find

$$\mathcal{E}_q^{\perp} = J_{\perp} q_{\perp}^2 + \Delta$$

for which reason

$$(\mathcal{E}_q^{\perp})^2 \cong 2 J_{\perp} \Delta q_{\perp}^2 + \Delta^2 \qquad \text{(A6.17)}$$

Combining (A6. 16) and (A6. 17) we find the connexions

$$\alpha\beta_\perp \triangleq J_\perp \Delta \tag{A6.18}$$

$$\Delta = \sqrt{\alpha^2 - \gamma^2} \tag{A6.19}$$

By means of the expressions of the dispersion relation constants and the energy we are able to carry out analytically the basal plane direction part of the integration of Δ M(T) and b(T). The c-direction part of the integration is carried out numerically on a computer. We find for Δ M(T):

$$\Delta M(T) = \frac{V_c}{S_1(2\pi)^3} 2\pi \int_0^{q_\parallel^{max}} \int_0^{q_\perp^{max}} \left[\frac{\alpha + \beta_\perp q_\perp^2 + \beta_\parallel q_\parallel^2}{\Delta + J_\perp q_\perp^2 + J_\parallel^{(2)} q_\parallel^2 + J_\parallel^{(4)} q_\parallel^4} \left(\frac{1}{e^{\epsilon_q / k_B T} - 1} + \frac{1}{2} \right) - \frac{1}{2} \right] dq_\parallel \, q_\perp \, dq_\perp \tag{A6.20}$$

Now we introduce the following short hand notation

$$C_1(q_\parallel) = \alpha + \beta_\parallel q_\parallel^2 \tag{A6.21}$$

$$C_2(q_\parallel) = \Delta + J_\parallel^{(2)} q_\parallel^2 + J_\parallel^{(4)} q_\parallel^4 \tag{A6.22}$$

and find

$$\Delta M(T) = \frac{V_c}{S_1(2\pi)^3} \Big\{ -\frac{\pi}{2} q_\parallel^{max} (q_\perp^{max})^2 + \pi \int_0^{q_\parallel^{max}} C_1(q_\parallel) I_1(q_\parallel) dq_\parallel + \pi\beta_\perp \int_0^{q_\parallel^{max}} I_2(q_\parallel) dq_\parallel + 2\pi \int_0^{q_\parallel^{max}} C_1(q_\parallel) I_3(q_\parallel) dq_\parallel + 2\pi\beta_\perp \int_0^{q_\parallel^{max}} I_4(q_\parallel) dq_\parallel \Big\} \tag{A6.23}$$

The integrals $I_1(q_\parallel)$, $I_2(q_\parallel)$, $I_3(q_\parallel)$ and $I_4(q_\parallel)$ are

$$I_1(q_\parallel) = \int_0^{q_\perp^{max}} \frac{1}{C_2(q_\parallel) + J_\perp q_\perp^2}\, q_\perp dq_\perp \tag{A6.24}$$

$$I_2(q_\parallel) = \int_0^{q_\perp^{max}} \frac{q_\perp^2}{C_2(q_\parallel) + J_\perp q_\perp^2}\, q_\perp dq_\perp \tag{A6.25}$$

$$I_3(q_\parallel) \cong \int_0^{\infty} \frac{1}{C_2(q_\parallel) + J_\perp q_\perp^2}\; \frac{1}{e^{[C_2(q_\parallel) + J_\perp q_\perp^2]/k_B T} - 1}\, q_\perp dq_\perp \tag{A6.26}$$

$$I_4(q_\parallel) \cong \int_0^{\infty} \frac{q_\perp^2}{C_2(q_\parallel) + J_\perp q_\perp^2}\; \frac{1}{e^{[C_2(q_\parallel) + J_\perp q_\perp^2]/k_B T} - 1}\, q_\perp dq_\perp \tag{A6.27}$$

They are found to terms linear in temperature

$$I_1(q_\parallel) = \frac{1}{2J_\perp} \ln\left(1 + \frac{J_\perp (q_\perp^{max})^2}{C_2(q_\parallel)}\right) \tag{A6.28}$$

$$I_2(q_\parallel) = \frac{1}{2J_\perp}\left[(q_\perp^{max})^2 - \frac{C_2(q_\parallel)}{J_\perp} \ln\left(1 + \frac{J_\perp (q_\perp^{max})^2}{C_2(q_\parallel)}\right)\right] \tag{A6.29}$$

$$I_3(q_\parallel) \cong \frac{1}{2J_\perp} \frac{k_B T}{C_2(q_\parallel)} \left\{ e^{-C_2(q_\parallel)/k_B T} + \frac{1}{2} e^{-2C_2(q_\parallel)/k_B T} + \frac{1}{3} e^{-3C_2(q_\parallel)/k_B T} \right\} \tag{A6.30}$$

$$I_4(q_\parallel) \cong 0 \tag{A6.31}$$

The other characteristic function b(T) is found to

$$\ell(T) = -\frac{V_c}{S_1(2\pi)^3}\, 2\pi\gamma \int_0^{q_{\parallel}^{max}} dq_{\parallel} \int_0^{q_{\perp}^{max}} \frac{1}{C_2(q_{\parallel}) + J_{\perp} q_{\perp}^2} \times$$

$$\times \left(\frac{1}{e^{[C_2(q_{\parallel}) + J_{\perp} q_{\perp}^2]/k_B T} - 1} + \frac{1}{2} \right) q_{\perp} dq_{\perp}$$

$$= -\frac{V_c}{S_1(2\pi)^3} \left\{ \gamma \frac{\pi}{2} \int_0^{q_{\parallel}^{max}} I_1(q_{\parallel})\, dq_{\parallel} + 2\pi\gamma \int_0^{q_{\parallel}^{max}} I_3(q_{\parallel})\, dq_{\parallel} \right\}$$

(A6.32)

Model no. 2: Quadratic q-Dependence of the Dispersion Relation in the c-Direction and Linear q-Dependence of the Dispersion Relation in the Basal Plane Direction

In this model we take in the basal plane direction

$$\mathcal{A}_q^{\perp} = \alpha + \beta_{\perp} q_{\perp} \qquad (A6.33)$$

$$\mathcal{B}_q = \gamma \qquad (A6.34)$$

$$\ell_q^{\perp} = \Delta + J_{\perp} q_{\perp} \qquad (A6.35)$$

In the c-direction we take the same expressions as in the first model. Therefore $\Delta M(T)$ is still expressable through (A6.23) but the integrals are replaced by

$$I_1'(q_{\parallel}) = \int_0^{q_{\perp}^{max}} \frac{1}{C_2(q_{\parallel}) + J_{\perp} q_{\perp}}\, dq_{\perp}\, q_{\perp} \qquad (A6.36)$$

$$I_2'(q_{\parallel}) = \int_0^{q_{\perp}^{max}} \frac{q_{\perp}}{C_2(q_{\parallel}) + J_{\perp} q_{\perp}}\, q_{\perp} dq_{\perp} \qquad (A6.37)$$

$$I_3'(q_\parallel) \cong \int_0^\infty \frac{1}{C_2(q_\parallel)+J_\perp q_\perp} \; \frac{1}{e^{[C_2(q_\parallel)+J_\perp q_\perp]/k_BT}-1} \; q_\perp \, dq_\perp \tag{A6.38}$$

$$I_4'(q_\parallel) \cong \int_0^\infty \frac{q_\perp}{C_2(q_\parallel)+J_\perp q_\perp} \; \frac{1}{e^{[C_2(q_\parallel)+J_\perp q_\perp]/k_BT}-1} \; q_\perp \, dq_\perp \tag{A6.39}$$

These sets of integrals are found to

$$I_1'(q_\parallel) = \frac{q_\perp^{max}}{J_\perp} - \frac{C_2(q_\parallel)}{J_\perp^2} \ln\left(1+\frac{J_\perp q_\perp^{max}}{C_2(q_\parallel)}\right) \tag{A6.40}$$

$$I_2'(q_\parallel) = \frac{1}{2}\frac{(q_\perp^{max})^2}{J_\perp} - \frac{C_2(q_\parallel)\, q_\perp^{max}}{J_\perp^2} + \frac{C_2(q_\parallel)^2}{J_\perp^3} \ln\left(1+\frac{J_\perp q_\perp^{max}}{C_2(q_\parallel)}\right) \tag{A6.41}$$

$$I_3'(q_\parallel) \cong 0 \tag{A6.42}$$

$$I_4'(q_\parallel) \cong \frac{(k_BT)^2}{J_\perp^3} \left\{ e^{-C_2(q_\parallel)/k_BT} + \frac{1}{2} e^{2C_2(q_\parallel)/k_BT} + \frac{1}{3} e^{3C_2(q_\parallel)/k_BT} \right\} \tag{A6.43}$$

b(Γ) is found to

$$b(T) = -\frac{V_c}{S_1(2\pi)^3} \left\{ \frac{\pi}{2}\gamma \int_0^{q_\parallel^{max}} I_1'(q_\parallel)\, dq_\parallel + 2\pi\gamma \int_0^{q_\parallel^{max}} I_3'(q_\parallel)\, dq_\parallel \right\} \tag{A6.44}$$

The purpose of setting up two alternative models is to be able to fit the measured dispersion relations as accurate as possible in a concrete calculation.

APPENDIX 7

The Spin Wave Dispersion Constants of a Hexagonal Closed Packed Lattice in a Basal Plane Representation

In section (5) we have set up a Hamiltonian of the heavy rare earth metals consisting of isotrope exchange, magneto crystalline anisotropy, magnetostriction and a term coming from an applied external magnetic field. Here we want to calculate the individual contributions from the total Hamiltonian to the spin wave dispersion relations that have two branches: An optical and an acoustical branch. From (5.82) and (5.83) we have for the dispersion relations:

$$\hbar\omega_K^{op} = \left\{ (\mathcal{A}_K + |\mathcal{C}_K|) + |\mathcal{B}_K| \right\}^{1/2} \times \left\{ (\mathcal{A}_K + |\mathcal{C}_K|) - |\mathcal{B}_K| \right\}^{1/2} \tag{A7.1}$$

$$\hbar\omega_K^{ac} = \left\{ (\mathcal{A}_K - |\mathcal{C}_K|) + |\mathcal{B}_K| \right\}^{1/2} \times \left\{ (\mathcal{A}_K - |\mathcal{C}_K|) - |\mathcal{B}_K| \right\}^{1/2} \tag{A7.2}$$

The constants A_K, B_K and C_K defined through the relation (5.14) are the dispersion constants. All terms of the Hamiltonian contribute to these characteristic constants of the spin wave energies.

The isotrop exchange

As mentioned in eq. (5.6), the isotrop exchange interaction of the hexagonal closed packed structure - built up from two interpenetrating hexagonal sublattices is

$$\mathcal{H}_{ex} = -\sum_{l>l'} \mathcal{J}(\bar{R}_{ll'})\, \underline{J}_l\cdot\underline{J}_{l'} - \sum_{m>m'} \mathcal{J}(\bar{R}_{mm'})\, \underline{J}_m\cdot\underline{J}_{m'} - \sum_{l,m} \mathcal{J}'(\bar{R}_{l,m})\, \underline{J}_l\cdot\underline{J}_m$$

$$= \mathcal{H}_{ex,1} + \mathcal{H}_{ex,2} + \mathcal{H}_{ex,3} \tag{A7.3}$$

$\mathcal{H}_{ex,1}$ and $\mathcal{H}_{ex,2}$ are equal and describe the intra sublattice exchange of the two sublattices constituting the hcp-lattice, whereas $\mathcal{H}_{ex,3}$ describes the intersublattice exchange. $\mathcal{H}_{ex,1}$ and $\mathcal{H}_{ex,2}$ are characterized by the exchange functions $\mathcal{J}(R_{ll'})$ and $\mathcal{J}(R_{mm'})$ respectively and $\mathcal{J}'(R_{lm})$ is the inter exchange function different from the intra exchange functions; Using table (1) we transform the exchange interactions to Bose operator expressions. We find

$$\mathcal{H}_{ex,1} = \sum_{l>l'} \mathcal{J}(\bar{R}_{ll'}) \Big[-S_1^2 + S_1 (a_l^+ a_l + a_{l'}^+ a_{l'} - a_l^+ a_{l'} - a_l a_{l'}^+) - a_l^+ a_l a_{l'}^+ a_{l'}$$
$$+ (S_1 - \sqrt{S_2}) \left(a_l^+ a_{l'}^+ a_{l'} a_{l'} + a_l^+ a_l^+ a_l a_{l'} + a_l a_{l'}^+ a_{l'}^+ a_{l'} + a_l^+ a_l a_l a_{l'}^+ \right)\Big] \tag{A7.4}$$

$$\mathcal{H}_{ex,2} = \sum_{m>m'} \mathcal{J}(\bar{R}_{mm'}) \Big(-S_1^2 + S_1 (b_m^+ b_m + b_{m'}^+ b_{m'} - b_m^+ b_{m'} - b_m b_{m'}^+) - b_m^+ b_m b_{m'}^+ b_{m'}$$
$$+ (S_1 - \sqrt{S_2}) \left(b_m^+ b_{m'}^+ b_{m'} b_{m'} + b_m^+ b_m^+ b_m b_{m'} + b_m b_{m'}^+ b_{m'}^+ b_{m'} + b_m^+ b_m b_m b_{m'}^+ \right)\Big] \tag{A7.5}$$

$$\mathcal{H}_{ex,3} = \sum_{l,m} \mathcal{J}(\bar{R}_{l,m}) \Big[-S_1^2 + S_1 \left(a_l^+ a_l + b_m^+ b_m - a_l^+ b_m - a_l b_m^+ \right) - a_l^+ a_l b_m^+ b_m$$
$$+ (S_1 - \sqrt{S_2}) \left(a_l^+ b_m^+ b_m b_m + a_l^+ a_l^+ a_l b_m + a_l b_m^+ b_m^+ b_m + a_l^+ a_l a_l b_m^+ \right) \Big] \qquad \text{(A 7.6)}$$

By use of the general formulae for Fourier transformation of Bose operators in table 8 we find for the non-interacting part of the exchange

$$(\mathcal{H}_{ex})_0 = -N \left(\mathcal{J}(0) + \mathcal{J}'(0) \right) J(J+1) + \sum_{\underline{K}} \Big\{ \tfrac{1}{2} S_1 \left(\mathcal{J}(0) - \mathcal{J}(\underline{K}) + \mathcal{J}'(0) \right) \left(a_K^+ a_K + a_K a_K^+ + b_K^+ b_K + b_K b_K^+ \right)$$
$$- S_1 \mathcal{J}'(\underline{K}) a_K^+ b_K - S_1 \mathcal{J}'(\underline{K})^* a_K b_K^+ \Big\}$$
$$= E_0(ex) + \sum_{\underline{K}} \Big\{ \tfrac{1}{2} A_K^a \left(a_K^+ a_K + a_K a_K^+ \right) + \tfrac{1}{2} A_K^b \left(b_K^+ b_K + b_K b_K^+ \right) + C_K a_K b_K^+ + C_K^* b_K a_K^+ \Big\}$$
$$\text{(A 7.7)}$$

and hence the contributions of the dispersion constants are

$$E_0(ex) = -N J(J+1) \left(\mathcal{J}(0) + \mathcal{J}'(0) \right) \qquad \text{(A 7.8)}$$

$$A_K^a(ex) = A_K^b(ex) = S_1 \left(\mathcal{J}(0) - \mathcal{J}(\underline{K}) + \mathcal{J}'(0) \right) \qquad \text{(A 7.9)}$$

$$C_K(ex) = -S_1 \mathcal{J}'(\underline{K})^* \qquad \text{(A 7.10)}$$

$$C_K^*(ex) = -S_1 \mathcal{J}'(k) \tag{A7.11}$$

A Fourier transformation of the interacting part gives, table 8:

$$\begin{aligned}
(\mathcal{H}_{ex})_1 = \frac{1}{2N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} & \left\{ 2(S_1 - \sqrt{S_2})\left(\mathcal{J}(\bar{q}_4) + \mathcal{J}(\bar{q}_1)\right) - \mathcal{J}(\bar{q}_4 - \bar{q}_2) \right\} \Big(a^+_{q_1} a^+_{q_2} a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4} + \\
& \qquad b^+_{q_1} b^+_{q_2} b_{q_3} b_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4} \Big) + \\
\frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} & \Big\{ [S_1 - \sqrt{S_2}] \Big[\mathcal{J}'(\bar{q}_2) b^+_{q_1} a^+_{q_2} b_{q_3} b_{q_4} + \mathcal{J}'(\bar{q}_2)^* a^+_{q_1} b^+_{q_2} a_{q_3} a_{q_4} + \\
& \qquad \mathcal{J}'(\bar{q}_4) a^+_{q_1} a^+_{q_2} a_{q_3} b_{q_4} + \mathcal{J}'(\bar{q}_4)^* b^+_{q_1} b^+_{q_2} b_{q_3} a_{q_4} \Big] \delta_{q_1+q_2,\, q_3+q_4} + \\
\frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} & \mathcal{J}'(\bar{q}_4 - \bar{q}_2) \, a^+_{q_1} b^+_{q_2} a_{q_3} b_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}
\end{aligned} \tag{A7.12}$$

The Hartree-Fock decoupling of the terms of the interacting exchange part has been carried out to give for the dispersion constants:

$$\Delta E_0(ex) = \frac{1}{2N}\sum_{k_1 k_2}\Big\{\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)-2(S_1-\sqrt{S_2})\big(3\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2)\big)\Big(\langle a^+_{k_1}a_{k_1}\rangle\langle a^+_{k_2}a_{k_2}\rangle+\langle b^+_{k_1}b_{k_1}\rangle\langle b^+_{k_2}b_{k_2}\rangle\Big)$$

$$+\frac{1}{2N}\sum_{k_1}\Big\{\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)-4(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2)\big)\Big)\ \big(\langle a^+_{k_1}a_{k_1}\rangle+\langle b^+_{k_1}b_{k_1}\rangle\big)$$

$$-2\sum_{k_2}\Big[(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)\langle a^+_{k_2}b_{k_2}\rangle+(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)^*\langle b^+_{k_2}a_{k_2}\rangle\Big]$$

$$-\frac{1}{N}\sum_{k_1 k_2}(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)\Big(2\langle b^+_{k_1}b_{k_1}\rangle\langle a^+_{k_2}b_{k_2}\rangle+\langle b^+_{-k_2}a^+_{k_2}\rangle\langle b_{k_1}b_{-k_1}\rangle\Big)$$

$$-\frac{1}{N}\sum_{k_1 k_2}(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)^*\Big(2\langle a^+_{k_1}a_{k_1}\rangle\langle b^+_{k_2}a_{k_2}\rangle+\langle a^+_{k_2}b^+_{-k_2}\rangle\langle a_{k_1}a_{-k_1}\rangle\Big)$$

$$-\frac{1}{N}\sum_{k_1 k_2}(S_1-\sqrt{S_2})\Big(2\,\mathcal{J}'(\underline{k}_2)\langle a^+_{k_1}a_{k_1}\rangle\langle a^+_{k_2}b_{k_2}\rangle+\mathcal{J}'(\underline{k}_2)^*\langle a^+_{-k_1}a^+_{k_1}\rangle\langle a_{k_2}b_{-k_2}\rangle\Big)$$

$$-\frac{1}{N}\sum_{k_1 k_2}(S_1-\sqrt{S_2})\Big(2\,\mathcal{J}'(\underline{k}_2)^*\langle b^+_{k_1}b_{k_1}\rangle\langle b^+_{k_2}a_{k_2}\rangle+\mathcal{J}(\underline{k}_2)^*\langle b^+_{-k_1}b^+_{k_1}\rangle\langle b_{-k_2}a_{k_2}\rangle\Big)$$

$$-\frac{1}{N}\sum_{k_1 k_2}\mathcal{J}'(0)\langle a^+_{k_1}a_{k_1}\rangle\langle b^+_{k_2}b_{k_2}\rangle-\frac{1}{N}\sum_{k_1 k_2}\mathcal{J}'(\underline{k}_1-\underline{k}_2)\Big(\langle a^+_{k_1}b_{k_1}\rangle\langle b^+_{k_2}a_{k_2}\rangle+\langle a^+_{k_1}b^+_{-k_1}\rangle\langle a_{k_2}b_{k_2}\rangle\Big)$$

$$-\frac{1}{2}\sum_{k_1}\mathcal{J}'(0)\big(\langle a^+_{k_1}a_{k_1}\rangle+\langle b^+_{k_1}b_{k_1}\rangle\big)-\frac{1}{2N}\sum_{k_1 k_2}\Big\{2(S_1-\sqrt{S_2})\big[\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2)\big]-\mathcal{J}(\underline{k}_1-\underline{k}_2)\Big\}\Big(\langle a^+_{k_1}a^+_{k_1}\rangle\langle a_{k_2}a_{k_2}\rangle$$

$$+\langle b^+_{k_1}b^+_{k_1}\rangle\langle b_{k_2}b_{k_2}\rangle\Big)$$

$$\Delta A^{a}_{k_1}(ex) = \frac{1}{N}\sum_{k_2}\Big\{\big[\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)-4(S_1-\sqrt{S_2})(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2))\big]\langle a^{+}_{k_2}a_{k_2}\rangle + \mathcal{J}'(0)\langle b^{+}_{k_2}b_{k_2}\rangle$$
$$+\,2(S_1-\sqrt{S_2})\big[\mathcal{J}'(\underline{k}_2)^{*}\langle b^{+}_{k_2}a_{k_2}\rangle + \mathcal{J}'(\underline{k}_2)\langle a^{+}_{k_2}b_{k_2}\rangle\big]\Big\} \tag{A7.14}$$

$$\Delta A^{b}_{k_1}(ex) = \frac{1}{N}\sum_{k_2}\Big\{\big[\mathcal{J}(0)+\mathcal{J}(\underline{k}_1-\underline{k}_2)-4(S_1-\sqrt{S_2})(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2))\big]\langle b^{+}_{k_2}b_{k_2}\rangle + \mathcal{J}'(0)\langle a^{+}_{k_2}a_{k_2}\rangle$$
$$+\,2(S_1-\sqrt{S_2})\big[\mathcal{J}'(\underline{k}_2)^{*}\langle b^{+}_{k_2}a_{k_2}\rangle + \mathcal{J}'(\underline{k}_2)\langle a^{+}_{k_2}b_{k_2}\rangle\big]\Big\} \tag{A7.15}$$

$$\Delta B^{a}_{k_2}(ex) = \frac{1}{N}\sum_{k_1}\Big\{\big[2(S_1-\sqrt{S_2})(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2))-\mathcal{J}(\underline{k}_1-\underline{k}_2)\big]\langle a^{+}_{k_1}a^{+}_{-k_1}\rangle + 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)^{*}\langle a^{+}_{k_2}b^{+}_{-k_2}\rangle\Big\} \tag{A7.16}$$

$$\Delta B^{b}_{k_2}(ex) = \frac{1}{N}\sum_{k_1}\Big\{\big[2(S_1-\sqrt{S_2})(\mathcal{J}(\underline{k}_1)+\mathcal{J}(\underline{k}_2))-\mathcal{J}(\underline{k}_1-\underline{k}_2)\big]\langle b^{+}_{k_1}b^{+}_{-k_1}\rangle + 2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)\langle b^{+}_{-k_1}a^{+}_{k_1}\rangle\Big\} \tag{A7.17}$$

$$\Delta C_{k_2}(ex) = \frac{1}{N}\sum_{k_1}\Big\{2(S_1-\sqrt{S_2})\,\mathcal{J}'(\underline{k}_2)^{*}\big(\langle a^{+}_{k_1}a_{k_1}\rangle + \langle b^{+}_{k_1}b_{k_1}\rangle\big) + \mathcal{J}'(\underline{k}_1-\underline{k}_2)\langle a^{+}_{k_1}b_{k_1}\rangle\Big\} \tag{A7.18}$$

$$\Delta D_{k_2}(ex) = \frac{1}{N}\sum_{k_1}\Big\{\mathcal{J}'(\underline{k}_1-\underline{k}_2)\langle a^{+}_{k_1}b^{+}_{-k_1}\rangle + (S_1-\sqrt{S_2})\big(\mathcal{J}'(\underline{k}_2)^{*}\langle b^{+}_{-k_1}b^{+}_{k_1}\rangle + \mathcal{J}'(\underline{k}_2)^{*}\langle a^{+}_{k_1}a^{+}_{-k_1}\rangle\big)\Big\} \tag{A7.19}$$

The single-ion anisotropy

In section (4) we have treated the single-ion anisotropy of a Bravais lattice. The hcp-lattice is built up from two hexagonal Bravais lattices, for which reason the single ion magneto crystalline anisotropy is equal in the two sub-lattices. Besides we want to deal with a hcp-lattice where the magnetization is lying in the basal plane. This requires a rotation of the anisotropy from a c-axis representation to a representation of the direction of magnetization. This operation is done by using the general rotation expressions of the Stevens operators set up in table 6 and putting the angle $\beta = \frac{\pi}{2}$;

In the c-axis representation the sublattice single-ion anisotropy is

$$\mathcal{H}_{an} = \sum_i \left\{ B_2^0 O_2^0(c) + B_4^0 O_4^0(c) + B_6^0 O_6^0(c) + B_6^6 O_6^6(c) \right\}_i \tag{A7.20}$$

After rotating the Stevens operators the sublattice anisotropy has become:

$$\begin{aligned}\mathcal{H}_{an} = \sum_i \Big\{ & B_2^0 \left[-\tfrac{1}{2} O_2^0(c) - \tfrac{3}{2} O_2^2(c) \right] + B_4^0 \left[\tfrac{3}{8} O_4^0(c) + \tfrac{5}{2} O_4^2(c) + \tfrac{35}{8} O_4^4(c) \right] \\ & + B_6^0 \left[-\tfrac{5}{16} O_6^0(c) - \tfrac{105}{32} O_6^2(c) - \tfrac{63}{16} O_6^4(c) - \tfrac{231}{32} O_6^6(c) \right] \\ & + B_6^6 \left[\tfrac{1}{16} O_6^0(c) - \tfrac{15}{32} O_6^2(c) + \tfrac{3}{16} O_6^4(c) - \tfrac{1}{32} O_6^6(c) \right] \cos 6\alpha \\ & - B_6^6 \left[\tfrac{3}{4} O_6^1(c) - \tfrac{5}{8} O_6^3(c) + \tfrac{3}{8} O_6^5(c) \right] \sin 6\alpha \Big\}_i \end{aligned} \tag{A7.21}$$

As shown in section (4) Stevens operators $O_K^q\binom{c}{s}$ with an odd q number do not contribute in a temperature calculation, therefore we only take terms consisting of an even number of Bose operators.

Again a Fourier transformation is carried out to give for the non-interacting part, by means of table 8

$$(\mathcal{H}_{an})_0 = N\left[-B_2^0 S_2\left(1+\frac{3}{2S_1}\right)+3B_4^0 S_4\left(1+\frac{5}{S_1}\right)-(5B_6^0-B_6^6\cos 6\alpha)S_6\left(1+\frac{21}{2}\frac{1}{S_1}\right)\right]$$

$$+\frac{1}{2}\left[3B_2^0\frac{S_2}{S_1}-30B_4^0\frac{S_4}{S_1}+21(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_1}\right]\sum_K\left(a_k^+a_k+a_ka_k^+\right)$$

$$+\frac{1}{2}\left[-3B_2^0\sqrt{S_2}+30B_4^0\frac{S_4}{\sqrt{S_2}}-15(7B_6^0+B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_2}}\right]\sum_K\left(a_k^+a_k^+ +a_ka_{-k}\right) \qquad (A7.22)$$

from which the contributions to the dispersion constants are immidiately read as

$$E_0(an) = N\left[-B_2^0 S_2\left(1+\frac{3}{2S_1}\right)+3B_4^0\left(1+\frac{5}{S_1}\right)-(5B_6^0-B_6^6\cos 6\alpha)S_6\left(1+\frac{21}{2S_1}\right)\right] \qquad (A7.23)$$

$$A_K^a(an) = \left[3B_2^0\frac{S_2}{S_1}-30B_4^0\frac{S_4}{S_1}+21(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_1}\right] \qquad (A7.24)$$

$$B_K^a(an) = \left[-3B_2^0\sqrt{S_2}+30B_4^0\frac{S_4}{\sqrt{S_2}}-15(7B_6^0+B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_2}}\right] \qquad (A7.25)$$

As the two sublattices are equal, the other one contributes with dispersion constants that are the same. Therefore E_0(an) must be taken once more and A_K^b(an) = A_K^a(an) and B_K^b(an) = B_K^a(an) where "b" means the other sublattice. A Fourier transformation of the interacting part of the sublattice anisotropy gives

$$
\begin{aligned}
(\mathcal{H}_{an})_1 = \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} \Big\{ & \Big[-\tfrac{3}{2} B_2^0 + \tfrac{135}{2} B_4^0 \frac{S_4}{S_2} - 105\,(5B_6^0 - B_6^6 \cos 6\alpha)\frac{S_6}{S_2}\Big]\, a^+_{q_1} a^+_{q_2} a_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4} \\
& + \sqrt{\frac{S_2}{S_1 S_3}} \Big[\tfrac{3}{2} B_2^0 \sqrt{S_2}\Big(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big) - 15 B_4^0 \frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big) \\
& \qquad + \tfrac{15}{2}(7 B_6^0 + B_6^6 \cos 6\alpha)\Big(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2}\Big)\frac{S_6}{\sqrt{S_2}} \Big] \times \\
& \qquad \big[a^+_{q_1} a^+_{q_2} a^+_{-q_3} a_{q_4} + a^+_{q_1} a_{-q_2} a_{q_3} a_{q_4} \big]\, \delta_{q_1+q_2,\, q_3+q_4} \\
& + \Big[\tfrac{35}{4} B_4^0 \sqrt{S_4} - \tfrac{15}{4}(21 B_6^0 - B_6^6 \cos 6\alpha)\frac{S_6}{\sqrt{S_4}} \Big] \times \\
& \quad \big[a^+_{q_1} a^+_{q_2} a^+_{-q_3} a^+_{-q_4} + a_{-q_1} a_{-q_2} a_{q_3} a_{q_4} \big]\, \delta_{q_1+q_2,\, q_3+q_4} \Big\} \qquad \text{(A7.26)}
\end{aligned}
$$

Doing a Hartree-Fock decoupling of the interacting anisotropy part we find the following contributions to the dispersion constants, by means of table 9

$$
\begin{aligned}
\Delta E_0(an) = \frac{1}{N} \Big[-\tfrac{3}{2} B_2^0 + \tfrac{135}{2} B_4^0 \frac{S_4}{S_2} - 105\,(5 B_6^0 - B_6^6 \cos 6\alpha)\frac{S_6}{S_2} \Big) \times \Big[& -2N \sum_{k_1} \big(\langle a^+_{k_1} a_{k_1} \rangle + \langle b^+_{k_1} b_{k_1} \rangle \big) \\
& + 2 \sum_{k_1 k_2} \big(\langle a^+_{k_1} a_{k_1} \rangle \langle a^+_{k_2} a_{k_2} \rangle + \langle b^+_{k_1} b_{k_1} \rangle \langle b^+_{k_2} b_{k_2} \rangle \big) \Big]
\end{aligned}
$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big[\frac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)-15B_4^0\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0+B_6^6\cos 6\alpha)\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\frac{S_6}{\sqrt{S_2}}\Big]\times$$

$$\times\Big[-\frac{3}{2}N\sum_{k_1}\big[\langle a_{k_1}^+a_{-k_1}\rangle+\langle b_{k_1}^+b_{-k_1}^+\rangle+\langle a_{k_1}a_{-k_1}\rangle+\langle b_{k_1}b_{-k_1}\rangle\big]$$

$$-3\sum_{k_1k_2}\big[\langle a_{k_2}^+a_{k_2}\rangle(\langle a_{k_1}^+a_{-k_1}\rangle+\langle a_{k_1}a_{-k_1}\rangle)+\langle b_{k_2}^+b_{k_2}\rangle(\langle b_{k_2}^+b_{-k_2}^+\rangle+\langle b_{k_2}b_{-k_2}\rangle)\big]\Big]$$

$$+\frac{1}{N}\Big[\frac{35}{4}B_4^0\sqrt{S_4}+\frac{15}{4}(21B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\Big]\times\Big[-3\sum_{k_1k_2}\big(\langle a_{k_1}^+a_{-k_1}^+\rangle\langle a_{k_2}^+a_{-k_2}^+\rangle+\langle a_{k_1}a_{-k_1}\rangle\langle a_{k_2}a_{-k_2}\rangle$$

$$+\langle b_{k_1}^+b_{-k_1}^+\rangle\langle b_{k_2}^+b_{-k_2}^+\rangle+\langle b_{k_1}b_{-k_1}\rangle\langle b_{k_2}b_{-k_2}\rangle\big)\Big]$$

(A7.27)

$$A_k^a(am)=\Big[-\frac{3}{2}B_2^0+\frac{135}{2}B_4^0\frac{S_4}{S_2}-105(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_2}\Big]\frac{4}{N}\sum_{k_1}\langle a_{k_1}^+a_{k_1}\rangle$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big(\frac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)-15B_4^0\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0+B_6^6\cos 6\alpha)\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\frac{S_6}{\sqrt{S_2}}\Big)3\sum_{k_1}\big(\langle a_{k_1}^+a_{-k_1}\rangle+\langle a_{k_1}a_{k_1}\rangle\big)$$

(A7.28)

$$A_K^b(am) = \left[-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105\left(5B_6^0 - B_6^6\cos 6\alpha\right)\frac{S_6}{S_2}\right]\frac{4}{N}\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$

$$+\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left[\frac{3}{2}B_2^0\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right.$$

$$\left.+\frac{15}{2}\left(7B_6^0 + B_6^6\cos 6\alpha\right)\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right]\cdot 3\sum_{K_1}\left(\langle b_{K_1}^+ b_{-K_1}^+\rangle + \langle b_{K_1} b_{-K_1}\rangle\right) \qquad \text{(A7.29)}$$

$$\Delta B_K^a(am) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\frac{3}{2}B_2^0\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right) - 15B_4^0\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\right.$$

$$\left.+\frac{15}{2}\left(7B_6^0 + B_6^6\cos 6\alpha\right)\left(6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right)\frac{S_6}{\sqrt{S_2}}\right)\cdot 6\sum_{K_1}\langle a_{K_1}^+ a_{K_1}\rangle$$

$$+\frac{1}{N}\left(\frac{35}{4}B_4^0\sqrt{S_4} - \frac{15}{4}\left(21B_6^0 - B_6^6\cos 6\alpha\right)\frac{S_6}{\sqrt{S_4}}\right)\cdot 12\sum_{K_1}\langle a_{K_1} a_{-K_1}\rangle$$

$$+\frac{1}{N}\left(-\frac{3}{2}B_2^0 + \frac{135}{2}B_4^0\frac{S_4}{S_2} - 105\left(5B_6^0 - B_6^6\cos 6\alpha\right)\frac{S_6}{S_2}\right)\cdot 2\sum_{K_1}\langle a_{K_1}^+ a_{-K_1}^+\rangle \qquad \text{(A7.30)}$$

$$\Delta B_K^b(am) = \frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\Big[\frac{3}{2}B_2^0\sqrt{S_2}\Big(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)-15B_4^0\frac{S_4}{\sqrt{S_2}}\Big(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)$$

$$+\frac{15}{2}(7B_6^0+B_6^6\cos 6\alpha)\Big(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\Big)\Big]\cdot 6\sum_{K_1}\langle b_{K_1}^+ b_{K_1}\rangle$$

$$+\frac{1}{N}\Big[\frac{35}{4}B_4^0\sqrt{S_4}-\frac{15}{4}(21B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{\sqrt{S_4}}\Big]\cdot 12\sum_{K_1}\langle b_{K_1} b_{K_1}\rangle$$

$$+\frac{1}{N}\Big[-\frac{3}{2}B_2^0+\frac{135}{2}B_4^0\frac{S_4}{S_2}-105(5B_6^0-B_6^6\cos 6\alpha)\frac{S_6}{S_2}\Big]\cdot 2\sum_{K}\langle b_{K_1}^+ b_{K_1}^+\rangle \qquad \text{(A7.31)}$$

<u>Single-ion magnetostriction</u>

In the thesis by Danielsen[23)] it has been shown in appendix 3 that the single-ion magnetostriction Hamiltonian for a hexagonal Bravais lattice in the c-axis representation might be expanded after the irreducible strains of the hexagonal point group.

This Hamiltonian expressed in Racah operators might be transformed into Stevens operators by use of the formulae (2.23)-(2.25) to give

$$\mathcal{H}_{me} = -\sum_{\ell}\Big\{(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})O_2^0(c)+(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})O_4^0(c)$$

$$+(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})O_6^0(c)+(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2})O_6^6(c)$$

$$+B_{22}^{\gamma}(\bar{\varepsilon}_1^{\gamma}O_2^2(c)+\bar{\varepsilon}_2^{\gamma}O_2^2(s))+B_{42}^{\gamma}(\bar{\varepsilon}_1^{\gamma}O_4^2(c)+\bar{\varepsilon}_2^{\gamma}O_4^2(s))$$

$$B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}O_6^2(c)+\bar{\varepsilon}_2^{\gamma}O_6^2(s)\right)+B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}O_4^4(c)+\bar{\varepsilon}_2^{\gamma}O_4^4(s)\right)$$

$$+B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}O_6^4(c)+\bar{\varepsilon}_2^{\gamma}O_6^4(s)\right)+B_{21}^{\varepsilon}\left(\bar{\varepsilon}_1^{\varepsilon}O_2^1(c)+\bar{\varepsilon}_2^{\varepsilon}O_2^1(s)\right)$$

$$+B_{41}^{\varepsilon}\left(\bar{\varepsilon}_1^{\varepsilon}O_4^1(c)+\bar{\varepsilon}_2^{\varepsilon}O_4^1(s)\right)+B_{61}^{\varepsilon}\left(\bar{\varepsilon}_1^{\varepsilon}O_6^1(c)+\bar{\varepsilon}_2^{\varepsilon}O_6^1(s)\right)$$

$$+B_{65}^{\varepsilon}\left(\bar{\varepsilon}_1^{\varepsilon}O_6^5(c)+\bar{\varepsilon}_2^{\varepsilon}O_6^5(s)\right) \tag{A7.32}$$

The B'^S are phenomenological magnetoelastic coupling constants. The irreducible strains are defined and explained in section (4). As we are dealing with a ferromagnetic structure with the magnetic moments in the hexagonal basal planes we again, as with the anisotropy, do a rotation operation on the Stevens operators to a representation of the direction of magnetization. By use of table 6 with the angle $\beta = \frac{\pi}{2}$ we find

$$\mathcal{H}_{me} = -\sum_{l}\Big\{\Big[\tfrac{1}{2}\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)-\tfrac{1}{2}B_{22}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right)\Big]O_2^0(c)$$

$$\Big[-\tfrac{3}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)+\tfrac{1}{8}B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right)$$

$$-\tfrac{1}{8}B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right)\Big]O_4^0(c)$$

$$+\Big[\tfrac{5}{16}\big(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)-\tfrac{1}{16}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\alpha$$

$$-\tfrac{1}{16}B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)+\tfrac{1}{16}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\big)\Big]\,O_6^0(c)$$

$$+\Big[\tfrac{3}{2}\big(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)+\tfrac{1}{2}B_{22}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)\Big]\,O_2^2(c)$$

$$+\Big[-\tfrac{5}{2}\big(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)+\tfrac{1}{2}B_{42}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)+\tfrac{1}{2}B_{44}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\big)\Big]\,O_4^2(c)$$

$$+\Big[-\tfrac{35}{8}\big(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)-\tfrac{7}{8}B_{42}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)-\tfrac{1}{8}B_{44}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\big)\Big]\,O_4^4(c)$$

$$+\Big[\tfrac{105}{32}\big(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)+\tfrac{15}{32}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\alpha$$

$$-\tfrac{17}{32}B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)+\tfrac{5}{32}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\big)\Big]\,O_6^2(c)$$

$$+\Big[\tfrac{63}{16}\big(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)-\tfrac{3}{16}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\alpha$$

$$-\tfrac{3}{16}B_{62}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha+\bar{\varepsilon}_2^{\gamma}\sin 2\alpha\big)-\tfrac{13}{16}B_{64}^{\gamma}\big(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha+\bar{\varepsilon}_2^{\gamma}\sin 4\alpha\big)\Big]\,O_6^4(c)$$

$$+\Big[\tfrac{231}{32}\big(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)+\tfrac{1}{32}\big(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1}+B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\big)\cos 6\alpha\Big]\,O_6^6(c) \qquad \text{(A7.33)}$$

Here the following restrictions have been introduced:

1) odd-valued Stevens operators have been skipped, as they do not contribute in a temperature calculation. This means that the ϵ_1^{ϵ} and ϵ_2^{ϵ} -strains are now excluded in that way.

2) even-valued s-Stevens operators are not included. It has been shown in section (4), that in a non-interacting temperature calculation they do not contribute. They are therefore even in an interacting theory of higher order than the even valued Stevens operators that are left in the rotated single-ion magnetoelastic Hamiltonian. Expressing the Stevens operators by their Bose expansions we find for the magneto striction Hamiltonian:

$$
\begin{aligned}
\mathcal{H}_{me} = & \left[\mathcal{K}_2^0 2 S_2 \left(1 + \frac{3}{2S_1}\right) + \mathcal{K}_4^0 8 S_4 \left(1 + \frac{5}{S_1}\right) + \mathcal{K}_6^0 16 S_6 \left(1 + \frac{27}{2S_1}\right) \right] \\
& - \left[\mathcal{K}_2^0 S_2 \frac{3}{S_1} + \mathcal{K}_4^0 S_4 \frac{40}{S_1} + \mathcal{K}_6^0 S_6 \frac{168}{S_1} \right] \sum_{\ell} (a_\ell^+ a_\ell + a_\ell a_\ell^+) \\
& + \left[\mathcal{K}_2^2 \sqrt{S_2} + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}} \right] \sum_{\ell} (a_\ell^+ a_\ell^+ + a_\ell a_\ell) \\
& + \left[3 \mathcal{K}_2^0 + 180 \frac{S_4}{S_2} \mathcal{K}_4^0 + 840 \frac{S_6}{S_2} \mathcal{K}_6^0 \right] \sum_{\ell} a_\ell^+ a_\ell^+ a_\ell a_\ell \\
& - \left[\mathcal{K}_2^2 \sqrt{S_2} \sqrt{\frac{S_2}{S_1 S_3}} \left(\sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) + \mathcal{K}_4^2 6 \frac{S_4}{\sqrt{S_2}} \sqrt{\frac{S_2}{S_1 S_3}} \left(\frac{7}{3} + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) + \mathcal{K}_6^2 16 \frac{S_6}{\sqrt{S_2}} \sqrt{\frac{S_2}{S_1 S_3}} \left(6 + \sqrt{\frac{S_1 S_3}{S_2}} - \frac{S_3}{S_2} \right) \right] \cdot \\
& \cdot \sum (a_\ell^+ a_\ell^+ a_\ell^+ a_\ell + a_\ell^+ a_\ell a_\ell a_\ell) + \\
& \left[\mathcal{K}_4^4 2 \sqrt{S_4} + \mathcal{K}_6^4 20 \frac{S_6}{\sqrt{S_4}} \right] \sum_{\ell} (a_\ell^+ a_\ell^+ a_\ell^+ a_\ell^+ + a_\ell a_\ell a_\ell a_\ell)
\end{aligned}
\tag{A7.34}
$$

where the constants $\mathcal{K}_K^q$ are given by

$$\mathcal{K}_2^0 = \frac{1}{2}\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{1}{2} B_{22}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) \tag{A7.35}$$

$$\mathcal{K}_4^0 = -\frac{3}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{1}{8} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) - \frac{1}{8} B_{44}^{\gamma}\left(\cos 4\alpha\,\bar{\varepsilon}_1^{\gamma} + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.36}$$

$$\mathcal{K}_6^0 = \frac{5}{16}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{1}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{1}{16} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) + \frac{1}{16} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.37}$$

$$\mathcal{K}_2^2 = \frac{3}{2}\left(B_{20}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{20}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{1}{2} B_{22}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) \tag{A7.38}$$

$$\mathcal{K}_4^2 = -\frac{5}{2}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{1}{2} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) + \frac{1}{2} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.39}$$

$$\mathcal{K}_6^2 = \frac{105}{32}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) + \frac{15}{32}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{17}{32} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) + \frac{5}{32} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.40}$$

$$\mathcal{K}_4^4 = -\frac{35}{8}\left(B_{40}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{40}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{7}{8} B_{42}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) - \frac{1}{8} B_{44}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.41}$$

$$\mathcal{H}_6^4 = \frac{63}{16}\left(B_{60}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{60}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right) - \frac{3}{16}\left(B_{66}^{\alpha,1}\bar{\varepsilon}^{\alpha,1} + B_{66}^{\alpha,2}\bar{\varepsilon}^{\alpha,2}\right)\cos 6\alpha$$
$$- \frac{3}{16} B_{62}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 2\alpha + \bar{\varepsilon}_2^{\gamma}\sin 2\alpha\right) - \frac{13}{16} B_{64}^{\gamma}\left(\bar{\varepsilon}_1^{\gamma}\cos 4\alpha + \bar{\varepsilon}_2^{\gamma}\sin 4\alpha\right) \tag{A7.42}$$

Proceeding in the same way as with the isotrop exchange and the single-ion anisotropy we do a Fourier transformation of the magnetostriction terms finding a non-interacting - and an interacting part;

Again it shall be remembered that the hcp-lattice is built up from two interpenetrating sublattices, for which reason the non-interacting contributions to the dispersion constants become:

$$E_0(me) = 2\mathcal{H}_2^0 S_2\left(1+\frac{3}{2S_1}\right) + 8 S_4 \mathcal{H}_4^0\left(1+\frac{5}{S_1}\right) + 16\,\mathcal{H}_6^0 S_6\left(1+\frac{21}{2S_1}\right) \tag{A7.43}$$

$$A_K^a(me) = -\left(6\mathcal{H}_2^0\frac{S_2}{S_1} + 80\,\mathcal{H}_4^0\frac{S_4}{S_1} + 336\mathcal{H}_6^0\frac{S_6}{S_1}\right) = A_K^b \tag{A7.44}$$

$$B_K^a(me) = 2\left(\mathcal{H}_2^2\sqrt{S_2} + \mathcal{H}_4^2\, 6\,\frac{S_4}{\sqrt{S_2}} + \mathcal{H}_6^2\; 16\,\frac{S_6}{\sqrt{S_2}}\right) = B_K^b \tag{A7.45}$$

Doing a Hartree-Fock decoupling of the interacting part by means of table 9 we find the contributions to the dispersion constants:

$$\Delta E_0(me) = \frac{1}{N}\left(3\mathcal{H}_2^0 + 180\,\frac{S_4}{S_2}\mathcal{H}_4^0 + 840\,\frac{S_6}{S_2}\mathcal{H}_6^0\right)\cdot\Big[-2N\sum_{K_1}\left(\langle a_{K_1}^+ a_{K_1}\rangle + \langle b_{K_1}^+ b_{K_1}\rangle\right)$$
$$- \sum_{K_1K_2}\left(2\langle a_{K_1}^+ a_{K_1}\rangle\langle a_{K_2}^+ a_{K_2}\rangle + \langle a_{K_1}^+ a_{-K_1}^+\rangle\langle a_{K_2} a_{-K_2}\rangle + 2\langle b_{K_1}^+ b_{K_1}\rangle\langle b_{K_2}^+ b_{K_2}\rangle + \langle b_{K_1}^+ b_{-K_1}^+\rangle\langle b_{K_2} b_{-K_2}\rangle\right)\Big]$$

$$+\frac{1}{N}\sqrt{\frac{s_2}{s_1 s_3}}\Big[\chi_2^2\sqrt{s_2}\Big(\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_4^2\, 6\frac{s_4}{\sqrt{s_2}}\Big(\frac{7}{3}+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_6^2\, 16\frac{s_6}{\sqrt{s_2}}\Big(6+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)\Big]\times$$

$$\cdot\Big[3\sum_{K_1K_2}\Big(\langle a^+_{K_1}a_{K_1}\rangle\big(\langle a^+_{K_2}a^+_{-K_2}\rangle+\langle a_{K_2}a_{-K_2}\rangle\big)+\langle b^+_{K_1}b_{K_1}\rangle\big(\langle b^+_{K_2}b^+_{-K_2}\rangle+\langle b_{K_2}b_{-K_2}\rangle\big)\Big)$$

$$+\frac{3}{2}N\sum_{K_1}\big(\langle a^+_{K_1}a^+_{-K_1}\rangle+\langle a_{K_1}a_{-K_1}\rangle+\langle b^+_{K_1}b^+_{-K_1}\rangle+\langle b_{K_1}b_{-K_1}\rangle\big)\Big]$$

$$-\frac{1}{N}\Big(\chi_4^4\, 2\sqrt{s_4}+\chi_6^4\, 20\frac{s_6}{\sqrt{s_4}}\Big)3\sum_{K_1K_2}\Big[\langle a^+_{K_1}a^+_{-K_1}\rangle\langle a^+_{K_2}a^+_{-K_2}\rangle+\langle a_{K_1}a_{-K_1}\rangle\langle a_{K_2}a_{-K_2}\rangle$$

$$+\langle b^+_{K_1}b^+_{-K_1}\rangle\langle b^+_{K_2}b^+_{-K_2}\rangle+\langle b_{K_1}b_{-K_1}\rangle\langle b_{K_2}b_{-K_2}\rangle\Big] \tag{A7.46}$$

$$\Delta A^a_K(me)=\Big(3\chi_2^0+180\frac{s_4}{s_2}\chi_4^0+840\frac{s_6}{s_2}\chi_6^0\Big)\frac{4}{N}\sum_{K_1}\langle a^+_{K_1}a_{K_1}\rangle$$

$$-\frac{1}{N}\sqrt{\frac{s_2}{s_1 s_3}}\Big(\chi_2^2\sqrt{s_2}\Big(\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_4^2\, 6\frac{s_4}{\sqrt{s_2}}\Big(\frac{7}{3}+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_6^2\, 16\frac{s_6}{\sqrt{s_2}}\Big(6+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)\Big)\times$$

$$3\sum_{K_1}\big(\langle a^+_{K_1}a^+_{-K_1}\rangle+\langle a_{K_1}a_{-K_1}\rangle\big) \tag{A7.47}$$

$$\Delta A^b_K(me)=\Big(3\chi_2^0+180\frac{s_4}{s_2}\chi_4^0+840\frac{s_6}{s_2}\chi_6^0\Big)\frac{4}{N}\sum_{K_1}\langle b^+_{K_1}b_{K_1}\rangle$$

$$-\frac{1}{N}\sqrt{\frac{s_2}{s_1 s_3}}\Big(\chi_2^2\sqrt{s_2}\Big(\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_4^2\, 6\frac{s_4}{\sqrt{s_2}}\Big(\frac{7}{3}+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)+\chi_6^2\, 16\frac{s_6}{\sqrt{s_2}}\Big(6+\sqrt{\frac{s_1 s_3}{s_2}}-\frac{s_3}{s_2}\Big)\Big)\times$$

$$3\sum_{K_1}\big(\langle b^+_{K_1}b^+_{-K_1}\rangle+\langle b_{K_1}b_{-K_1}\rangle\big) \tag{A7.48}$$

$$\Delta B_K^a(me) = -\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\mathcal{K}_2^2\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)+\mathcal{K}_4^2\,6\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)+\mathcal{K}_6^2\,16\frac{S_6}{\sqrt{S_2}}\left(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)\right)6\sum_{K_1}\langle a_{K_1}^+a_{K_1}\rangle$$

$$+\frac{1}{N}\left(\mathcal{K}_4^4\,2\sqrt{S_4}+\mathcal{K}_6^4\,20\frac{S_6}{\sqrt{S_4}}\right)12\sum_{K_1}\langle a_{K_1}a_{-K_1}\rangle$$

$$+\frac{1}{N}\left(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\right)2\sum_{K_1}\langle a_{K_1}^+a_{-K_1}^+\rangle \tag{A7.49}$$

$$\Delta B_K^b(me) = -\frac{1}{N}\sqrt{\frac{S_2}{S_1S_3}}\left(\mathcal{K}_2^2\sqrt{S_2}\left(\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)+\mathcal{K}_4^2\,6\frac{S_4}{\sqrt{S_2}}\left(\frac{7}{3}+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)+\mathcal{K}_6^2\,16\frac{S_6}{\sqrt{S_2}}\left(6+\sqrt{\frac{S_1S_3}{S_2}}-\frac{S_3}{S_2}\right)\right)6\sum_{K}\langle b_{K_1}^+b_{K_1}\rangle$$

$$+\frac{1}{N}\left(\mathcal{K}_4^4\,2\sqrt{S_4}+\mathcal{K}_6^4\,20\frac{S_6}{\sqrt{S_4}}\right)12\sum_{K_1}\langle b_{K_1}b_{-K_1}\rangle$$

$$+\frac{1}{N}\left(3\mathcal{K}_2^0+180\frac{S_4}{S_2}\mathcal{K}_4^0+840\frac{S_6}{S_2}\mathcal{K}_6^0\right)2\sum_{K_1}\langle b_{K_1}^+b_{-K_1}^+\rangle \tag{A7.50}$$

<u>Applied magnetic field</u>

Applying an external magnetic field in the basal plane we have the following Zeemann contributions to the Hamiltonian of the hcp-lattice, built up from two interpenetrating sublattices

$$\mathcal{H}_{zee} = -g\mu_B\sum_{\ell}\underline{H}\cdot\underline{J}_\ell - g\mu_B\sum_{m}\underline{H}\cdot\underline{J}_m \tag{A7.51}$$

$$H = (H_\xi, H_\eta, H_\zeta) = \left(H\cos(\alpha+\delta),\ H\sin(\alpha+\delta),\ 0\right) \tag{A7.52}$$

giving for the products

$$\underline{H}\cdot\underline{J}_\ell = H_\xi J_\ell^\xi + H_\eta J_\ell^\eta$$
$$\underline{H}\cdot\underline{J}_m = H_\xi J_m^\xi + H_\eta J_m^\eta \qquad (A7.53)$$

From the theory of rotation of Racah operators by Danielsen and Lindgård[8] we find the expressions for the angular momenta in the (ξ, η, ζ) coordinate system expressed by the angular momenta in the (x, y, z) coordinate system.

$$J_\xi = -\sin\alpha\, J_x + \cos\alpha\, J_y = \sin\alpha \frac{1}{\sqrt{2}}(\tilde{O}_{11} - \tilde{O}_{1,-1}) + \cos\alpha \frac{i}{\sqrt{2}}(\tilde{O}_{1,1} + \tilde{O}_{1,-1})$$

$$J_\eta = J_z = \tilde{O}_{10} \qquad (A7.54)$$

$$J_\zeta = \cos\alpha\, J_x + \sin\alpha\, J_y = -\cos\alpha \frac{1}{\sqrt{2}}(\tilde{O}_{1,1} - \tilde{O}_{1,-1}) + \sin\alpha \frac{i}{\sqrt{2}}(\tilde{O}_{1,1} + \tilde{O}_{1,-1})$$

and we end up with, when doing a Bose operator transformation and taking only into account an even number of Bose operators,

$$\underline{H}\cdot\underline{J}_\ell = H \sin(\alpha+\delta)\, J_\ell^z = H \sin(\alpha+\delta)\,(S_1 - a_\ell^+ a_\ell) \qquad (A7.55)$$
$$\underline{H}\cdot\underline{J}_m = H \sin(\alpha+\delta)\, J_m^z = H \sin(\alpha+\delta)\,(S_1 - b_m^+ b_m)$$

therefore

$$
\begin{aligned}
\mathcal{H}_{Zee} = & -g\mu_B H \sin(\alpha+\delta) \sum_{l} (S_1 - a_l^+ a_l) \\
& -g\mu_B H \sin(\alpha+\delta) \sum_{m} (S_1 - b_m^+ b_m) \\
= & -2g\mu_B H N S_1 \sin(\alpha+\delta) + g\mu_B H \sin(\alpha+\delta) \sum_{l} a_l^+ a_l + g\mu_B H \sin(\alpha+\delta) \sum_{m} b_m^+ b_m \\
= & -2\, g\mu_B H N \sin(\alpha+\delta)\, (S_1 + \tfrac{1}{2}) \\
& + g\mu_B H \sin(\alpha+\delta) \Big[\sum_{l} \tfrac{1}{2} (a_l^+ a_l + a_l a_l^+) + \sum_{m} \tfrac{1}{2} (b_m^+ b_m + b_m b_m^+) \Big]
\end{aligned}
\tag{A7.56}
$$

Doing a Fourier transformation we find the following contributions to the dispersion constants of the spin waves of the hcp-lattice

$$E_0(Zee) = -2g\mu_B H N \sin(\alpha+\delta) (S_1 + \tfrac{1}{2}) \tag{A7.57}$$

$$A_k^a(Zee) = g\mu_B H \sin(\alpha+\delta) = A_k^b(Zee) \tag{A7.58}$$

APPENDIX 8

The Characteristic Thermal Mean Values of the hcp-lattice

The renormalization calculation of the spin waves of the hexagonal closed packed structure of the heavy rare earth metals sets up some characteristic thermal mean values(appendix 7) through which the renormalized dispersion constants are expressed as a function of temperature. Therefore the following thermal mean values are calculated

$$\langle a_k^+ a_k \rangle, \ \langle b_k^+ b_k \rangle, \ \langle a_k a_{-k} \rangle, \ \langle a_{-k}^+ a_k^+ \rangle,$$

$$\langle b_k b_{-k} \rangle, \ \langle b_{-k}^+ b_k^+ \rangle, \ \langle a_k b_k^+ \rangle, \ \langle b_k a_k^+ \rangle,$$

$$\langle a_k b_{-k} \rangle, \ \langle b_{-k}^+ a_k^+ \rangle \tag{A8.1}$$

The Boseoperators "a" describe the one sublattice of the hcp-lattice and the Boseoperators "b" describe the other sublattice. "Mixed" thermal mean values containing both an "a" and a "b" - Bose operators come from the inter sublattice exchange part of the Hamiltonian of the system.

Following Kowalska and Lindgård[26] we transform the thermal mean values into Bose operators that are in the diagonal representation of the system. We find immediately the transformations from "old" to "new" Bose operators

$$a_k = p_0 F_k - m_0^* F_{-k}^+ + p_a G_k - m_a^* G_k^+ \tag{A8.2}$$

$$a_{-k}^+ = -m_0 F_k + p_0 F_{-k}^+ - m_a G_k + p_a G_k^+ \tag{A8.3}$$

$$b_k = c p_0 F_k - c m_0^* F_{-k}^+ - c p_a G_k + c m_a^* G_{-k}^+ \tag{A8.4}$$

$$b_{-k}^+ = -c m_0 F_k + c p_0 F_{-k}^+ + c m_a G_k - c p_a G_{-k}^+ \tag{A8.5}$$

F_K, F_K^+, G_K, G_K^+ are defined in connection with the diagonal Hamiltonian H_{diag} in equation (5.81). They obey the Bose commutation relations. The expansion coefficients of the transformations are, Kowalska and Lindgård[2f)]

$$m_s = \frac{B_K}{|B_K|}\left\{\frac{(\varepsilon_{Ks}^2 + |B_K|^2)^{1/2} - \varepsilon_{Ks}}{4\varepsilon_{Ks}}\right\}^{1/2} \tag{A8.6}$$

$$p_s = \left\{\frac{(\varepsilon_{Ks}^2 + |B_K|^2)^{1/2} + \varepsilon_{Ks}}{4\varepsilon_{Ks}}\right\}^{1/2} \tag{A8.7}$$

$$C = \frac{\mathcal{C}_K}{|\mathcal{C}_K|} \tag{A8.8}$$

s = (o, a) (o: optic; a: acoustic)

Forming the thermal mean values of (A8.1) by means of the transformations (A8.2) - (A8.5), we find

$$\langle a_K^+ a_K\rangle = \Big\{ (p_o^2 + |m_o|^2)\langle n_K^o\rangle + (p_a^2 + |m_a|^2)\langle n_K^a\rangle + (|m_o|^2 + |m_a|^2)\Big\} \tag{A8.9}$$

$$\langle b_K^+ b_K\rangle = |C|^2 \langle a_K^+ a_K\rangle \tag{A8.10}$$

$$\langle a_{\underline{K}}^+ a_K^+\rangle = -\Big\{ 2m_o p_o\langle n_K^o\rangle + 2m_a p_a\langle n_K^a\rangle + m_o p_o + m_a p_a\Big\} \tag{A8.11}$$

$$\langle a_K a_{\underline{K}}\rangle = -\Big\{ 2m_o^* p_o\langle n_K^o\rangle + 2m_a^* p_a\langle n_K^a\rangle + m_o^* p_o + m_a^* p_a\Big\} \tag{A8.12}$$

$$\langle b_{-K}^{+} b_{K}^{+} \rangle = |c|^2 \langle a_{-K}^{+} a_{K}^{+} \rangle \tag{A8.13}$$

$$\langle b_{K} b_{-K} \rangle = |c|^2 \langle a_{K} a_{-K} \rangle \tag{A8.14}$$

$$\langle a_{K} b_{K}^{+} \rangle = c^{*} (p_o^2 + |m_o|^2) \langle n_K^o \rangle - c^{*} (p_a^2 + |m_a|^2) \langle n_K^a \rangle + c^{*} (p_o^2 - p_a^2) \tag{A8.15}$$

$$\langle b_{K} a_{K}^{+} \rangle = c (p_o^2 + |m_o|^2) \langle n_K^o \rangle - c (p_a^2 + |m_a|^2) \langle n_K^a \rangle + c (|m_o|^2 - |m_a|^2) \tag{A8.16}$$

$$\langle a_{K} b_{-K} \rangle = -2c^{*} m_o^{*} p_o \langle n_K^o \rangle + 2c^{*} m_a^{*} p_a \langle n_K^a \rangle + c^{*} (m_a^{*} p_a - m_o^{*} p_o) \tag{A8.17}$$

$$\langle b_{-K}^{+} a_{K}^{+} \rangle = -2c\, m_o p_o \langle n_K^o \rangle + 2c\, m_a p_a \langle n_K^a \rangle + c (m_a p_a - m_o p_o) \tag{A8.18}$$

The Bose factors $\langle n_K^o \rangle$ and $\langle n_K^a \rangle$ are given by

$$\langle n_K^o \rangle = \frac{1}{e^{\varepsilon_{K,o}/k_B T} - 1} \tag{A8.19}$$

$$\langle n_K^a \rangle = \frac{1}{e^{\varepsilon_{K,a}/k_B T} - 1} \tag{A8.20}$$

where the renormalized energy expressions of the optical- and acoustical branches are from (5.82) and (5.83)

$$\varepsilon_{K,o} = \left\{ (A_K + |C_K|)^2 - |B_K|^2 \right\}^{1/2} \tag{A8.21}$$

$$\varepsilon_{K,a} = \left\{ (A_K - |C_K|)^2 - |B_K|^2 \right\}^{1/2} \tag{A8.22}$$

A_K, B_K and C_K are the dispersion constants of the hcp-lattice spin waves calculated in appendix 7. By means of (A8.6), (A8.7) and (A8.8) we find the combinations of the expansion coefficients necessary to calculate the thermal mean values in (A8.9) - (A8.18)

$$p_o^2 + |m_o|^2 = \frac{A_K + |C_K|}{2\varepsilon_{K,o}} \tag{A8.23}$$

$$p_a^2 + |m_a|^2 = \frac{A_K - |C_K|}{2\varepsilon_{K,a}} \tag{A8.24}$$

$$m_o^2 + m_a^2 = \frac{A_K + |C_K|}{4\varepsilon_{K,o}} + \frac{A_K - |C_K|}{4\varepsilon_{K,a}} - \frac{1}{2} \tag{A8.25}$$

$$2 m_o p_o = \frac{B_K}{2\varepsilon_{K,o}} ; \quad 2 m_o^* p_o = \frac{B_K^*}{2\varepsilon_{K,o}} \tag{A8.26}$$

$$2 m_a p_a = \frac{B_K}{2\varepsilon_{K,a}} ; \quad 2 m_a^* p_a = \frac{B_K^*}{2\varepsilon_{K,a}} \tag{A8.27}$$

$$m_a p_a \pm m_o p_o = \frac{B_K}{4}\left(\frac{1}{\varepsilon_{K,a}} \pm \frac{1}{\varepsilon_{K,o}} \right) \tag{A8.28}$$

$$m_a^* p_a \pm m_o^* p_o = \frac{B_K^*}{4}\left(\frac{1}{\varepsilon_{K,a}} \pm \frac{1}{\varepsilon_{K,o}} \right) \tag{A8.29}$$

$$|m_o|^2 - |m_a|^2 = \frac{A_K + |C_K|}{4\varepsilon_{K,o}} - \frac{A_K - |C_K|}{4\varepsilon_{K,a}} \tag{A8.30}$$

$$p_o^2 - p_a^2 = \frac{A_K + |C_K|}{4\varepsilon_{K,o}} - \frac{A_K - |C_K|}{4\varepsilon_{K,a}} \tag{A8.31}$$

Therefore we finally find the characteristic thermal mean values

$$\langle a_K^+ a_K \rangle = \frac{A_K + |C_K|}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) + \frac{A_K - |C_K|}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) - \tfrac{1}{2} \tag{A8.32}$$

$$\langle b_K^+ b_K \rangle = \frac{C_K C_K^*}{|C_K|^2} \langle a_K^+ a_K \rangle \tag{A8.33}$$

$$\langle a_{-K}^+ a_K^+ \rangle = -\left[\frac{B_K}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) + \frac{B_K}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right] \tag{A8.34}$$

$$\langle a_K a_{-K} \rangle = -\left[\frac{B_K^*}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) + \frac{B_K^*}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right] \tag{A8.35}$$

$$\langle b_{-K}^+ b_K^+ \rangle = \frac{C_K C_K^*}{|C_K|^2} \langle a_{-K}^+ a_K^+ \rangle \tag{A8.36}$$

$$\langle b_K b_{-K} \rangle = \frac{C_K C_K^*}{|C_K|^2} \langle a_K a_{-K} \rangle \tag{A8.37}$$

$$\langle a_K b_K^+ \rangle = \frac{C_K^*}{|C_K|} \left\{ \frac{A_K + |C_K|}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) - \frac{A_K - |C_K|}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right\} \tag{A8.38}$$

$$\langle b_K a_K^+ \rangle = \frac{C_K}{|C_K|} \left\{ \frac{A_K + |C_K|}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) - \frac{A_K - |C_K|}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right\} \tag{A8.39}$$

$$\langle a_K b_{-K} \rangle = \frac{C_K^*}{|C_K|} \left\{ - \frac{B_K^*}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) + \frac{B_K^*}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right\} \tag{A8.40}$$

$$\langle b_{-K}^+ a_K^+ \rangle = \frac{C_K}{|C_K|} \left\{ - \frac{B_K}{2E_{K0}} \left(\langle n_K^0 \rangle + \tfrac{1}{2} \right) + \frac{B_K}{2E_{KA}} \left(\langle n_K^A \rangle + \tfrac{1}{2} \right) \right\} \tag{A8.41}$$

APPENDIX 9

The Macroscopic Anisotropy Energy of a Hexagonal Ferromagnetic Crystal

In (7.1) it is shown that the free energy of a hexagonal crystal contains an anisotropy part determined by

$$\mathcal{F}(\alpha_1,\alpha_2,\alpha_3) = K_0(T) + K_1(T)(\alpha_1^2+\alpha_2^2) + K_2(T)(\alpha_1^2+\alpha_2^2)^2 + K_3(T)(\alpha_1^2+\alpha_2^2)^3 + K_4(T)(\alpha_1^2-\alpha_2^2)(\alpha_1^4-14\alpha_1^2\alpha_2^2+\alpha_2^2) + \cdots \tag{A9.1}$$

to the 6^{th} order in the direction cosines of the magnetization. The direction cosines are characterized by the equation

$$\alpha_1^2+\alpha_2^2+\alpha_3^2 = 1 \tag{A9.2}$$

Now we want to transform the anisotropy energy from a dependence on the direction cosines to a dependence on the spherical angles (θ, φ).
They are connected through the relations:

$$\alpha_1 = \cos\alpha = \sin\theta\cos\varphi \tag{A9.3}$$

$$\alpha_2 = \cos\beta = \sin\theta\sin\varphi \tag{A9.4}$$

$$\alpha_3 = \cos\gamma = \cos\theta \tag{A9.5}$$

we immedeately find

$$\alpha_1^2+\alpha_2^2+\alpha_3^2 = \sin^2\theta(\cos^2\varphi+\sin^2\varphi)+\cos^2\theta = 1 \tag{A9.6}$$

Now look at the direction cosines expressions of the magneto crystalline energy:

$$\alpha_1^2+\alpha_2^2 = 1-\alpha_3^2 = 1-\cos^2\theta = \sin^2\theta \tag{A9.7}$$

$$(\alpha_1^2-\alpha_2^2)(\alpha_1^4-14\alpha_1^2\alpha_2^2+\alpha_2^4)=$$

$$\sin^6\theta(\cos^2\varphi-\sin^2\varphi)(\cos^4\varphi-14\cos^2\varphi\sin^2\varphi+\sin^4\varphi)$$

$$=\sin^6\theta\cos 6\varphi \tag{A9.8}$$

as

$$\cos 6\varphi=(\cos^2\varphi-\sin^2\varphi)(\cos^4\varphi-14\cos^2\varphi\sin^2\varphi+\sin^4\varphi) \tag{A9.9}$$

therefore we find

$$\mathcal{F}(\theta,\varphi)=K_0(T)+K_1(T)\sin^2\theta+K_2(T)\sin^4\theta+K_3(T)\sin^6\theta$$
$$+K_4(T)\sin^6\theta\cos 6\varphi+\dots \tag{A9.10}$$

This expression defines the anisotropy constants. However, instead of expanding the anisotropic free energy as in (A9.10) it might be given as an expansion after general surface harmonics $\mathcal{Y}_{2n}(\theta,\varphi)$, Birss[31].

$$\mathcal{F}(\theta,\varphi)=\sum_{n=0}^{\infty}\mathcal{Y}_{2n}(\theta,\varphi)=\sum_{n=0}^{\infty}\sum_{m=-2n}^{2n}\chi_{2n,m}\mathcal{Y}_{2n,m}(\theta,\varphi) \tag{A9.11}$$

for which reason

$$\mathcal{F}(\theta,\varphi)=\chi_{0,0}\mathcal{Y}_{0,0}+\chi_{2,0}\mathcal{Y}_{2,0}+\chi_{4,0}\mathcal{Y}_{4,0}+\chi_{6,0}\mathcal{Y}_{6,0}+\chi_{6,6}\mathcal{Y}_{6,6} \tag{A9.12}$$

$\mathcal{Y}_{n,o}$ are the zonal harmonics and $\mathcal{Y}_{n,m}$ are the tesseral harmonics. Harmonics of odd degree are absent because $\mathcal{F}(\theta,\varphi)=\mathcal{F}(\pi-\theta,\pi+\varphi)$.

Now

$$\mathcal{Y}_{0,0} = P_0^0(\cos\theta) = 1 \tag{A9.13}$$

$$\mathcal{Y}_{2,0} = P_2^0(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1) \tag{A9.14}$$

$$\mathcal{Y}_{4,0} = P_4^0(\cos\theta) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3) \tag{A9.15}$$

$$\mathcal{Y}_{6,0} = P_6^0(\cos\theta) = \frac{1}{16}(231\cos^6\theta - 315\cos^4\theta + 105\cos^2\theta - 5) \tag{A9.16}$$

$$\mathcal{Y}_{6,6} = \frac{1}{10395}\cos 6\varphi \, P_6^6(\cos\theta) = \sin^6\theta(\cos^2\varphi - \sin^2\varphi)(\cos^4\varphi - 14\cos^2\varphi\sin^2\varphi + \sin^4\varphi) \tag{A9.17}$$

where $P_l^m(\cos\theta)$ are the Legendre function.

The expansion coefficients $\mathcal{X}_{n,m}$ are known as the anisotropy coefficients in the expansion

$$T(\theta,\varphi) = \mathcal{X}_{0,0} + \mathcal{X}_{2,0}P_2^0(\cos\theta) + \mathcal{X}_{4,0}P_4^0(\cos\theta) + \mathcal{X}_{6,0}P_6^0(\cos\theta) + \mathcal{X}_{6,6}\sin^6\theta\cos 6\varphi + \ldots \tag{A9.18}$$

We now calculate the connexion between the anisotropy constants and the anisotropy coefficients, using the formulae

$$\cos^2\theta = 1 - \sin^2\theta \tag{A9.19}$$

$$\cos^4\theta = 1 - 2\sin^2\theta + \sin^4\theta \tag{A9.20}$$

$$\cos^6\theta = 1 - 3\sin^2\theta + 3\sin^4\theta - \sin^6\theta \tag{A9.21}$$

From (A9.14), (A9.15) and (A9.16) we find

$$\sin^2\theta = \frac{2}{3}\left(1 - P_2^0(\cos\theta)\right) \tag{A9.22}$$

$$\sin^4\theta = \frac{8}{35}\left(P_4^0(\cos\theta) - \frac{10}{3}P_2^0(\cos\theta) + \frac{7}{3}\right) \tag{A9.23}$$

$$\sin^6\theta = -\frac{16}{231}\left(P_6^0(\cos\theta) - \frac{189}{35}P_4^0(\cos\theta) + 11P_2^0(\cos\theta) - \frac{33}{5}\right) \tag{A9.24}$$

Putting these values into equation (A9.10) we find

$$\begin{aligned} T(\theta,\varphi) = {} & K_1(T)\left[\frac{2}{3} - \frac{2}{3}P_2^0(\cos\theta)\right] \\ & + K_2(T)\left[\frac{8}{35}P_4^0(\cos\theta) - \frac{16}{21}P_6^0(\cos\theta) + \frac{8}{15}\right] \\ & + K_3(T)\left[-\frac{16}{231}P_6^0(\cos\theta) + \frac{144}{385}P_4^0(\cos\theta) - \frac{16}{21}P_2^0(\cos\theta) + \frac{16}{35}\right] \\ & + K_4(T) \quad \cos 6\varphi \sin^6\theta \end{aligned} \tag{A9.25}$$

Comparing with equation (A9.18) we find the connexion

$$\chi_{0,0}(T) = \frac{2}{105}\left(35K_1(T) + 28K_2(T) + 24K_3(T)\right) \tag{A9.26}$$

$$\chi_{2,0}(T) = -\frac{2}{21}\left(7K_1(T) + 8K_2(T) + 8K_3(T)\right) \tag{A9.27}$$

$$\chi_{4,0}(T) = \frac{8}{385}\left(11K_2(T) + 18K_3(T)\right) \tag{A9.28}$$

$$\chi_{6,0}(T) = -\frac{16}{231}K_3(T) \tag{A9.29}$$

$$\chi_{6,6}(T) = K_4(T) \tag{A9.30}$$

REFERENCES

1) K.W.H. Stevens, Proc. Phys. Soc. A65 (1952) 209-215.

2) G. Racah, Phys. Rev. 62 (1942) 438-462.

3) A.R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton University Press, Princeton, 1957). 146 pp.

4) E. Jahnke and F. Emde, Tables of Functions with Formulae and Curves (Dover, New York, 1945). 380 pp.

5) H.A. Buckmaster, Can. J. Phys. 40 (1962) 1670-1677.

6) D. Smith and J.H.M. Thornley, Proc. Phys. Soc. 89(1966) 779-781.

7) H.A. Buckmaster, R. Chatterjee and Y.H. Shing, Phys. Stat. Sol. (a) 13, (1972) 9-50.

8) O. Danielsen and P.A. Lindgård, Risö Report No. 259 (1972) (Danish Atomic Energy Commission, Risö, DK 4000 Roskilde, Denmark). 93 pp.

9) M.T. Hutchings, Sol. State Phys. 16 (1964) 227-273.

10) R.J. Birgeneau, Can. J. Phys. 45 (1967) 3761-3771.

11) B.R. Judd, Operator Techniques in Atomic Spectroscopy (Mc-Graw-Hill, New York, 1963). 242 pp.

12) M. Rothenberg, R. Bivins, N. Metropolis and J.K. Wooten, The 3j- and 6j-symbols (Massachusetts Institute of Technology, Cambridge, Mass., [illegible] 498 pp.

13) H.C. Fogedby, Lecture Notes in Advanced Statistical Mechanics (1972) (Københavns Universitet, H.C. Ørsted Instituttet, Universitetsparken 2200 København N, Denmark) 137 pp.

14) T. Holstein and H. Primakoff, Phys. Rev. 58 (1940) 1098-1113.

15) S.V. Tyablikov, Methods in the Quantum Theory of Magnetism (Plenum Press, New York, 1967). 354 pp.

16) W. Marshall and S.W. Lovesey, Theory of Thermal Neutron Scattering (Claredon Press, Oxford, 1971). 599 pp.

17) F.J. Dyson, Phys. Rev. 102, (1956) 1217-1229.
F.J. Dyson, Phys. Rev. 102, (1956) 1230-1244.

18) T. Oguchi, Progr. Theoret. Phys. (Kyoto) 25 (1961) 721-722.

19) B.R. Cooper, R.J. Elliott, S.J. Nettel and H. Suhl, Phys. Rev. 127 (1962) 57-68.

20) D.A. Goodings and B.W. Southern, Can J. Phys 49(1971) 1139-1161.

21) R.J. Elliott and K.W.H. Stevens, Proc. Roy. Soc. A219 (1953) 387-404.

22) E. Callen and H. Callen, Phys. Rev. 139 (1965) A455-A471.

23) O. Danielsen, Thesis, Technical University of Denmark (1970).

24) E.A. Turov and V.G. Shavrov, Sovjet Phys. - Solid State 7 (1965) 166-172.

25) B.R. Cooper, Phys. Rev. 169 (1968) 281-294.

26) A. Kowalska and P.A. Lindgård, Risö Report No. 127 (1966)(Danish Atomic Energy Commission, Risö, DK 4000 Roskilde, Denmark). 30 pp.

27) H.B. Callen and E. Callen, J. Phys. Chem. Sol. 27 (1966) 1271-1285.

28) A.R. Mackintosh and H.B. Møller, Magnetic Properties of Rare Earth Metals (Plenum Press, London and New York, 1972). 5, 187-244. 425 pp.

29) H.B. Møller, J.C.G. Houmann, J. Jensen and A.R. Mackintosh, Neutron Inelastic Scattering 1972
Proceedings of a Symposium Grenoble 6-10 March 1972, IAEA, Vienna, 1972. 603-610.

30) J. Smitt and H.G. Beljers, Philips Res. Rept. 10 (1955) 113-130.

31) R.R. Birss, Symmetry and Magnetism (North-Holland Publishing Company, Amsterdam, 1964) pp.

32) M.S.S. Brooks, D.A. Goodings and H.I. Ralph, J. Phys. C 1 (1968) 132-145.

33) M.S.S. Brooks, J. Phys. C 2 (1969) 1016-1022.

34) M.S.S. Brooks, Phys. Rev. B1, (1970) 2257-2264.

35) T. Egami, J. Phys. C 5 (1972) L85-L88.

36) M.S.S. Brooks and T. Egami, J. Phys. C 6 (1973) 513-531.

37) H.B. Møller, J.C.G. Houmann, M. Nielsen and A.R. Mackintosh, Magnetic Properties of Rare Earth Metals (Plenum Press, London and New York, 1972). 425 pp. 5 187-244.

38) D.E. Hegland, S. Legvold and F.H. Spedding, Phys. Rev. 131, (1963) 158-162.

39) R.J. Elliott and K.W.H. Stevens, Proc. Roy. Soc. A218 (1953) 553-566.

40) A.J. Freeman and R.E. Watson, Phys. Rev. 127 (1962) 2058-2075.

41) J. J. Rhyne and S. Legvold, Phys. Rev. 138, (1965) A507-A514.

42) F. I. Darnell, Phys. Rev. 132, (1963) 1098-1100.

43) R. J. Elliott, Phys. Rev. 124, (1961) 346-353.

44) J. L. Fèron, G. Huy and R. Panthenet, Les Elements des Terres Rares II 17 (Coloques Inter. du C.R.N.S. N^{o} 180, 1970).

45) J. J. Rhyne, S. Foner, E. J. McNiff and R. J. Doclo, J. Appl. Phys 39 (1968) 892-893.

46) J. J. Rhyne and A. E. Clark, J. Appl. Phys. 38 (1967) 1379-1380.

47) J. L. Stanford and R. C. Young, Phys. Rev. 157 (1967) 245-251.

48) K. Tajima and S. Chikazumi, J. Phys. Soc. Japan, 23 (1967) 1175.

49) R. Z. Levitin and B. K. Peromarev, Sovjet Phys.-JETP, 26 (1968) 1121-1122.

50) P. H. Bly, W. D. Corner and K. N. R. Raylor, J. Appl. Phys. 39 (1968) 1336-1338.

51) P. DeV. Du Plessis, Physica, 41 (1969) 379-388.

TABLES

Table 1

Racah operator equivalents

$X = J(J+1)$

$$\tilde{O}_{0,0} = 1$$

$$\tilde{O}_{1,0} = J_z$$

$$\tilde{O}_{1,\pm1} = \mp\sqrt{\tfrac{1}{2}}\,J^{\pm}$$

$$\tilde{O}_{2,0} = \tfrac{1}{2}\Big[3J_z^2 - X\Big]$$

$$\tilde{O}_{2,\pm1} = \mp\sqrt{\tfrac{3}{2}}\,\tfrac{1}{2}\Big[J_zJ^{\pm} + J^{\pm}J_z\Big]$$

$$\tilde{O}_{2,\pm2} = \sqrt{\tfrac{3}{8}}\,(J^{\pm})^2$$

$$\tilde{O}_{3,0} = \tfrac{1}{2}\Big[5J_z^3 - (3X-1)\,J_z\Big]$$

$$\tilde{O}_{3,\pm1} = \mp\sqrt{\tfrac{3}{16}}\,\tfrac{1}{2}\Big[(5J_z^2 - X - \tfrac{1}{2})J^{\pm} + J^{\pm}\,(\cdots)\Big]$$

$$\tilde{O}_{3,\pm2} = \sqrt{\tfrac{15}{8}}\,\tfrac{1}{2}\Big[J_z(J^{\pm})^2 + (J^{\pm})^2J_z\Big]$$

$$\tilde{O}_{3,\pm3} = \mp\sqrt{\tfrac{5}{16}}\,(J^{\pm})^3$$

$$\tilde{O}_{4,0} = \tfrac{1}{8}\Big[35J_z^4 - (30X-25)\,J_z^2 + 3X^2 - 6X\Big]$$

$$\tilde{O}_{4,\pm1} = \mp\sqrt{\tfrac{5}{16}}\,\tfrac{1}{2}\Big[(7J_z^3 - (3X+1)J_z)J^{\pm} + J^{\pm}(\cdots)\Big]$$

$$\tilde{O}_{4,\pm2} = \sqrt{\tfrac{5}{32}}\,\tfrac{1}{2}\Big[(7J_z^2 - X - 5)(J^{\pm})^2 + (J^{\pm})^2(\cdots)\Big]$$

$$\tilde{O}_{4,\pm3} = \mp\sqrt{\tfrac{35}{16}}\,\tfrac{1}{2}\Big[J_z(J^{\pm})^3 + (J^{\pm})^3J_z\Big]$$

$$\tilde{O}_{4,\pm4} = \sqrt{\tfrac{35}{128}}\,(J^{\pm})^4$$

$$\tilde{O}_{5,0} = \tfrac{1}{8}\Big[63J_z^5 - (70X-105)J_z^3 + (15X^2 - 50X + 12)\,J_z\Big]$$

$$\tilde{O}_{5,\pm1} = \mp\sqrt{\tfrac{15}{128}}\,\tfrac{1}{2}\Big[(21J_z^4 - 14XJ_z^2 + X^2 - X + \tfrac{3}{2})J^{\pm} + J^{\pm}(\cdots)\Big]$$

$$\tilde{O}_{5,\pm2} = \sqrt{\tfrac{105}{32}}\,\tfrac{1}{2}\Big[(3J_z^3 - (X+6)J_z)(J^{\pm})^2 + (J^{\pm})^2\,(\cdots)\Big]$$

$$\tilde{O}_{5,\pm3} = \mp\sqrt{\tfrac{35}{256}}\,\tfrac{1}{2}\Big[(9J_z^2 - X - \tfrac{33}{2})(J^{\pm})^3 + (J^{\pm})^3(\cdots)\Big]$$

$$\tilde{O}_{5,\pm4} = \sqrt{\tfrac{315}{128}}\,\tfrac{1}{2}\Big[J_z(J^{\pm})^4 + (J^{\pm})^4J_z\Big]$$

$$\tilde{O}_{5,\pm5} = \mp\sqrt{\tfrac{63}{256}}\,(J^{\pm})^5$$

$$\tilde{O}_{6,0} = \frac{1}{16}\left[231\,J_z^6 - (315\,X - 735)\,J_z^4 + (105\,X^2 - 525\,X + 294)\,J_z^2 - 5\,X^3 + 40\,X^2 - 60\,X\right]$$

$$\tilde{O}_{6,\pm1} = \mp\sqrt{\frac{21}{128}}\,\frac{1}{2}\left[(33\,J_z^5 - (30\,X - 15)\,J_z^3 + (5\,X^2 - 10\,X + 12)\,J_z)\,J^\pm + J^\pm(\cdots)\right]$$

$$\tilde{O}_{6,\pm2} = \sqrt{\frac{105}{1024}}\,\frac{1}{2}\left[(33\,J_z^4 - (18\,X + 123)\,J_z^2 + X^2 + 10\,X + 102)\,(J^\pm)^2 + (J^\pm)^2(\cdots)\right]$$

$$\tilde{O}_{6,\pm3} = \mp\sqrt{\frac{105}{256}}\,\frac{1}{2}\left[(11\,J_z^3 - (3\,X + 59)\,J_z)\,(J^\pm)^3 + (J^\pm)^3(\cdots)\right]$$

$$\tilde{O}_{6,\pm4} = \sqrt{\frac{63}{512}}\,\frac{1}{2}\left[(11\,J_z^2 - X - 38)\,(J^\pm)^4 + (J^\pm)^4(\cdots)\right]$$

$$\tilde{O}_{6,\pm5} = \mp\sqrt{\frac{693}{256}}\,\frac{1}{2}\left[J_z(J^\pm)^5 + (J^\pm)^5 J_z\right]$$

$$\tilde{O}_{6,\pm6} = \sqrt{\frac{231}{1024}}\,(J^\pm)^6$$

$$\tilde{O}_{7,0} = \frac{1}{16}\left[429\,J_z^7 - (693\,X - 2310)\,J_z^5 + (315\,X^2 - 2205\,X + 3213)\,J_z^3 - (35\,X^3 - 385\,X^2 + 882\,X - 180)\,J_z\right]$$

$$\tilde{O}_{7,\pm1} = \mp\sqrt{\frac{7}{32\,768}}\,\frac{1}{2}\left[(1716\,J_z^6 - (1980\,X - 2310)\,J_z^4 + (540\,X^2 - 1880\,X + 2184)\,J_z^2 - (20\,X^3 - 130\,X^2 + 270\,X + 225))\,J^\pm + J^\pm(\cdots)\right]$$

$$\tilde{O}_{7,\pm2} = \sqrt{\frac{21}{1024}}\,\frac{1}{2}\left[(143\,J_z^5 - (110\,X + 325)\,J_z^3 + (15\,X^2 + 170\,X + 2033)\,J_z)\,(J^\pm)^2 + (J^\pm)^2(\cdots)\right]$$

$$\tilde{O}_{7,\pm3} = \mp\sqrt{\frac{21}{16\,384}}\,\frac{1}{2}\left[(286\,J_z^4 - (132\,X + 2992)\,J_z^2 + 6\,X^2 + 222\,X + 3400)\,(J^\pm)^3 + (J^\pm)^3(\cdots)\right]$$

$$\tilde{O}_{7,\pm4} = \sqrt{\frac{231}{512}}\,\frac{1}{2}\left[(13\,J_z^3 - (3\,X + 139)\,J_z)\,(J^\pm)^4 + (J^\pm)^4(\cdots)\right]$$

$$\tilde{O}_{7,\pm5} = \mp\sqrt{\frac{231}{2048}}\,\frac{1}{2}\left[(13\,J_z^2 - X - \frac{165}{2})\,(J^\pm)^5 + (J^\pm)^5(\cdots)\right]$$

$$\tilde{O}_{7,\pm6} = \sqrt{\frac{3003}{1024}}\,\frac{1}{2}\left[J_z(J^\pm)^6 + (J^\pm)^6 J_z\right]$$

$$\tilde{O}_{7,\pm7} = \mp\sqrt{\frac{429}{2048}}\,(J^\pm)^7$$

$$\tilde{O}_{8,0} = \frac{1}{128}\Big[6435\,J_z^8 - (12012\,X - 40040)\,J_z^6 + (6930\,X^2 - 60060\,X + 93555)\,J_z^4 -$$
$$(1260\,X^3 - 16270\,X^2 + 50388\,X - 37380)\,J_z^2 + 35\,X^4 - 700\,X^3 + 3780\,X^2 - 5040\,X\Big]$$

$$\tilde{O}_{8,\pm1} = \mp\sqrt{\frac{9}{2048}}\,\frac{1}{2}\left[(715\,J_z^7 - (1001\,X - 2002)\,J_z^5 + (385\,X^2 - 1925\,X + 2695)\,J_z^3 - (35\,X^3 - 315\,X^2 + 854\,X + 372)\,J_z)(J^\pm) + (J^\pm)(\cdots)\right]$$

$$\tilde{O}_{8,\pm2} = \sqrt{\frac{315}{8192}}\,\frac{1}{2}\left[(143\,J_z^6 - (143\,X + 1144)\,J_z^4 + (33\,X^2 + 407\,X + 5951)\,J_z^2 - (X^3 + 19\,X^2 + 372\,X + 4800))(J^\pm)^2 + (J^\pm)^2(\cdots)\right]$$

$$\tilde{O}_{8,\pm3} = \mp\sqrt{\frac{231}{2048}}\,\frac{1}{2}\left[(39\,J_z^5 - (26\,X + 663)\,J_z^3 + (3\,X^2 + 128\,X + 3648)\,J_z)(J^\pm)^3 + (J^\pm)^3(\cdots)\right]$$

$$\tilde{O}_{8,\pm4} = \sqrt{\frac{693}{16\,384}}\,\frac{1}{2}\left[(65\,J_z^4 - (26\,X + 1313)\,J_z^2 + X^2 + 66\,X + 4296)(J^\pm)^4 + (J^\pm)^4(\cdots)\right]$$

$$\tilde{O}_{8,\pm5} = \mp\sqrt{\frac{9009}{2048}}\,\frac{1}{2}\left[(5\,J_z^3 - (X + 80)\,J_z)(J^\pm)^5 + (J^\pm)^5(\cdots)\right]$$

$$\tilde{O}_{8,\pm6} = \sqrt{\frac{429}{8192}}\,\frac{1}{2}\left[(15\,J_z^2 - X - 123)(J^\pm)^6 + (J^\pm)^6(\cdots)\right]$$

$$\tilde{O}_{8,\pm7} = \mp\sqrt{\frac{6435}{2048}}\,\frac{1}{2}\left[J_z(J^\pm)^7 + (J^\pm)^7 J_z\right]$$

$$\tilde{O}_{8,\pm8} = \sqrt{\frac{6435}{32\,768}}\,(J^\pm)^8$$

Table 2
Stevens operator equivalents

$X = J(J+1)$

$$O_2^0(c) = 2 \quad \tilde{O}_{20} \quad = 3J_z^2 - X$$

$$O_2^2(c) = \frac{2}{\sqrt{3}}\frac{1}{\sqrt{2}}(\tilde{O}_{2,-2} + \tilde{O}_{2,2}) \quad = \frac{1}{2}\left[(J^+)^2 + (J^-)^2\right]$$

$$O_4^0(c) = 8 \quad \tilde{O}_{40} \quad = 35J_z^4 - \{30X - 25\}J_z^2 + 3X^2 - 6X$$

$$O_4^2(c) = \frac{4}{\sqrt{5}}\frac{1}{\sqrt{2}}(\tilde{O}_{4,-2} + \tilde{O}_{4,2}) \quad = \frac{1}{4}\left[\{7J_z^2 - X - 5\}\left[(J^+)^2 + (J^-)^2\right] + \left[(J^+)^2 + (J^-)^2\right]\{\cdots\}\right]$$

$$O_4^4(c) = \frac{8}{\sqrt{35}}\frac{1}{\sqrt{2}}(\tilde{O}_{4,-4} + \tilde{O}_{4,4}) \quad = \frac{1}{2}\left[(J^+)^4 + (J^-)^4\right]$$

$$O_6^0(c) = 16 \quad \tilde{O}_{60} \quad = 231J_z^6 - \{315X - 735\}J_z^4 + \{105X^2 - 525X + 294\}J_z^2 - 5X^3 + 40X^2 - 60X$$

$$O_6^2(c) = \frac{32}{\sqrt{210}}\frac{1}{\sqrt{2}}(\tilde{O}_{6,-2} + \tilde{O}_{6,2}) \quad = \frac{1}{4}\left[\{33J_z^4 - (18X + 123)J_z^2 + X^2 + 10X + 102\}\left[(J^+)^2 + (J^-)^2\right] + \left[(J^+)^2 + (J^-)^2\right]\{\cdots\}\right]$$

$$O_6^4(c) = \frac{16}{3\sqrt{7}}\frac{1}{\sqrt{2}}(\tilde{O}_{6,-4} + \tilde{O}_{6,4}) \quad = \frac{1}{4}\left[\{11J_z^2 - X - 38\}\left[(J^+)^4 + (J^-)^4\right] + \left[(J^+)^4 + (J^-)^4\right]\{\cdots\}\right]$$

$$O_6^6(c) = \frac{32}{\sqrt{462}}\frac{1}{\sqrt{2}}(\tilde{O}_{6,-6} + \tilde{O}_{6,6}) \quad = \frac{1}{2}\left[(J^+)^6 + (J^-)^6\right]$$

$$O_8^0(c) = 128 \quad \tilde{O}_{80} \quad = 6435J_z^8 - \{12012X - 54054\}J_z^6 + \{6930X^2 - 64680X + 95\,995\}J_z^4$$
$$+ \{-1260X^3 + 18270X^2 - 59388X + 21\,390\}J_z^2$$
$$+ 35X^4 - 700X^3 + 3780X^2 - 5040X$$

$$O_8^2(c) = \frac{64}{3\sqrt{70}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-2} + \tilde{O}_{8,2}) \quad = \frac{1}{4}\left[\{143J_z^6 - (143X + 1144)J_z^4 + (33X^2 + 407X + 5951)J_z^2\right.$$
$$\left. - (X^3 + 13X^2 + 372X + 4806)\}\left[(J^+)^2 + (J^-)^2\right] + \left[(J^+)^2 - (J^-)^2\right]\{\cdots\}\right]$$

$$O_8^4(c) = \frac{64}{3\sqrt{77}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-4} + \tilde{O}_{8,4}) \quad = \frac{1}{4}\left[\{65J_z^4 - (26X + 1313)J_z^2 + X^2 + 86X + 4284\}\left[(J^+)^4 + (J^-)^4\right] + \left[(J^+)^4 + (J^-)^4\right]\{\cdots\}\right]$$

$$O_8^6(c) = \frac{64}{\sqrt{858}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-6} + \tilde{O}_{8,6}) \quad = \frac{1}{4}\left[\{15J_z^2 - X - 123\}\left[(J^+)^6 + (J^-)^6\right] + \left[(J^+)^6 + (J^-)^6\right]\{\cdots\}\right]$$

$$O_8^8(c) = \frac{128}{3\sqrt{715}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-8} + \tilde{O}_{8,8}) \quad = \frac{1}{2}\left[(J^+)^8 + (J^-)^8\right]$$

Table 3

Coefficients relating Stevens operators to Racah operators

l	m	K_l^m	$\dfrac{\sqrt{\frac{2l+1}{4\pi}}}{K_l^m}$
1	0	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$	1
1	1	$\frac{1}{2}\sqrt{\frac{3}{\pi}}$	1
2	0	$\frac{1}{4}\sqrt{\frac{5}{\pi}}$	2
2	1	$\frac{1}{2}\sqrt{\frac{15}{\pi}}$	$\frac{1}{\sqrt{3}}$
2	2	$\frac{1}{4}\sqrt{\frac{15}{\pi}}$	$\frac{2}{\sqrt{3}}$
3	0	$\frac{1}{4}\sqrt{\frac{7}{\pi}}$	2
3	1	$\frac{1}{8}\sqrt{\frac{42}{\pi}}$	$\frac{4}{\sqrt{6}}$
3	2	$\frac{1}{4}\sqrt{\frac{105}{\pi}}$	$\frac{2}{\sqrt{15}}$
3	3	$\frac{1}{8}\sqrt{\frac{70}{\pi}}$	$\frac{4}{\sqrt{10}}$
4	0	$\frac{1}{16}\sqrt{\frac{9}{\pi}}$	8
4	1	$\frac{3}{8}\sqrt{\frac{10}{\pi}}$	$\frac{4}{\sqrt{10}}$
4	2	$\frac{3}{8}\sqrt{\frac{5}{\pi}}$	$\frac{4}{\sqrt{5}}$
4	3	$\frac{3}{8}\sqrt{\frac{70}{\pi}}$	$\frac{4}{\sqrt{70}}$
4	4	$\frac{3}{16}\sqrt{\frac{35}{\pi}}$	$\frac{8}{\sqrt{35}}$
5	0	$\frac{1}{16}\sqrt{\frac{11}{\pi}}$	8
5	1	$\frac{1}{16}\sqrt{\frac{165}{\pi}}$	$\frac{8}{\sqrt{15}}$
5	2	$\frac{1}{8}\sqrt{\frac{1155}{\pi}}$	$\frac{4}{\sqrt{105}}$
5	3	$\frac{1}{32}\sqrt{\frac{770}{\pi}}$	$\frac{16}{\sqrt{70}}$
5	4	$\frac{3}{16}\sqrt{\frac{385}{\pi}}$	$\frac{8}{3\sqrt{35}}$
5	5	$\frac{3}{32}\sqrt{\frac{154}{\pi}}$	$\frac{16}{3\sqrt{14}}$
6	0	$\frac{1}{32}\sqrt{\frac{13}{\pi}}$	16
6	1	$\frac{1}{16}\sqrt{\frac{273}{\pi}}$	$\frac{8}{\sqrt{21}}$
6	2	$\frac{1}{64}\sqrt{\frac{2730}{\pi}}$	$\frac{32}{\sqrt{210}}$
6	3	$\frac{1}{32}\sqrt{\frac{2730}{\pi}}$	$\frac{16}{\sqrt{210}}$
6	4	$\frac{3}{32}\sqrt{\frac{91}{\pi}}$	$\frac{16}{3\sqrt{7}}$
6	5	$\frac{3}{32}\sqrt{\frac{2002}{\pi}}$	$\frac{16}{3\sqrt{154}}$
6	6	$\frac{1}{64}\sqrt{\frac{6006}{\pi}}$	$\frac{32}{\sqrt{462}}$
7	0	$\frac{1}{32}\sqrt{\frac{15}{\pi}}$	16
7	1	$\frac{1}{256}\sqrt{\frac{105}{\pi}}$	$\frac{128}{\sqrt{7}}$
7	2	$\frac{3}{64}\sqrt{\frac{70}{\pi}}$	$\frac{32}{\sqrt{42}}$
7	3	$\frac{3}{128}\sqrt{\frac{35}{\pi}}$	$\frac{64}{\sqrt{21}}$
7	4	$\frac{3}{256}\sqrt{\frac{35}{\pi}}$	$\frac{128}{\sqrt{21}}$
7	5	$\frac{3}{128}\sqrt{\frac{770}{\pi}}$	$\frac{64}{\sqrt{462}}$
7	6	$\frac{3}{64}\sqrt{\frac{10,010}{\pi}}$	$\frac{32}{\sqrt{6006}}$
7	7	$\frac{21}{64}\sqrt{\frac{715}{\pi}}$	$\frac{32}{7\sqrt{429}}$
8	0	$\frac{1}{256}\sqrt{\frac{17}{\pi}}$	128
8	1	$\frac{3}{64}\sqrt{\frac{17}{\pi}}$	$\frac{32}{3}$
8	2	$\frac{3}{128}\sqrt{\frac{1190}{\pi}}$	$\frac{64}{3\sqrt{70}}$
8	3	$\frac{1}{64}\sqrt{\frac{19,635}{\pi}}$	$\frac{32}{\sqrt{1155}}$
8	4	$\frac{3}{128}\sqrt{\frac{1309}{\pi}}$	$\frac{64}{3\sqrt{77}}$
8	5	$\frac{3}{64}\sqrt{\frac{17,017}{\pi}}$	$\frac{32}{3\sqrt{1001}}$
8	6	$\frac{1}{128}\sqrt{\frac{14,586}{\pi}}$	$\frac{64}{\sqrt{858}}$
8	7	$\frac{3}{64}\sqrt{\frac{12,155}{\pi}}$	$\frac{32}{3\sqrt{715}}$
8	8	$\frac{3}{256}\sqrt{\frac{12,155}{\pi}}$	$\frac{128}{3\sqrt{715}}$

Table 4

Racah operator equivalents expanded in Bose operators

$$S_n = J(J-\tfrac{1}{2})(J-1)\cdots(J-\tfrac{n-1}{2})$$

$$\tilde{O}_{00} = 1$$

$$\tilde{O}_{10} = S_1\left[1 - \frac{1}{S_1}\, a^+a\right]$$

$$\tilde{O}_{11} = -\sqrt{S_1}\left[a - \frac{1}{\sqrt{S_2}}\left[\sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{1}{2}\left(1 + \sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$$

$$\tilde{O}_{20} = S_2\left[1 - \frac{3}{S_1}\, a^+a + \frac{3}{2S_2}\, a^+a^+aa\right]$$

$$\tilde{O}_{21} = -\sqrt{3}\,\frac{S_2}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[1 + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{1}{\sqrt{S_2}}\left(1 - \frac{\sqrt{S_1S_3}}{S_2}\right) + \frac{1}{2}\left(1 + \sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$$

$$\tilde{O}_{22} = \frac{\sqrt{6}}{2}\sqrt{S_2}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$$

$$\tilde{O}_{30} = S_3\left[1 - \frac{6}{S_1}\, a^+a + \frac{15}{2S_2}\, a^+a^+aa + \cdots\right]$$

$$\tilde{O}_{31} = -\sqrt{6}\,\frac{S_3}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[\frac{3}{2} + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{5}{2}\left[\frac{1}{2}\left(\frac{S_1}{S_2}\right) + \frac{1}{\sqrt{S_2}}\left(1 - \frac{\sqrt{S_1S_3}}{S_2}\right)\right] + \frac{1}{2}\left(1 + \sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$$

$$\tilde{O}_{32} = \frac{\sqrt{30}}{2}\,\frac{S_3}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[1 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$$

$$\tilde{O}_{33} = -\frac{\sqrt{10}}{2}\sqrt{S_3}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[\sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$$

$$\tilde{O}_{40} = S_4\left[1 - \frac{10}{S_1}\, a^+a + \frac{45}{2S_2}\, a^+a^+aa + \cdots\right]$$

$$\tilde{O}_{41} = -\sqrt{10}\,\frac{S_4}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[\frac{9}{2} + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{9}{2}\left[\frac{7}{6}\cdot\left(\frac{S_1}{S_2}\right) + \frac{1}{\sqrt{S_2}}\left(1 - \frac{\sqrt{S_1S_3}}{S_2}\right)\right] + \frac{1}{2}\left(1 + \sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$$

$$\tilde{O}_{42} = \frac{3\sqrt{10}}{2}\,\frac{S_4}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$$

$$\tilde{O}_{43} = -\frac{\sqrt{70}}{2}\,\frac{S_4}{\sqrt{S_3}}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[1 + \sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$$

$$\tilde{O}_{44} = \frac{\sqrt{70}}{4}\sqrt{S_4}\, aaaa + \cdots$$

$\tilde{a}_{30} = S_3\left[1 - \frac{15}{S_1}a^+a + \frac{105}{2S_2}a^+a^+aa + \cdots\right]$

$\tilde{a}_{31} = -\sqrt{15}\frac{S_3}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[7 + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[7\left[2 - (\frac{S_1}{S_2}) + \frac{1}{\sqrt{S_2}}(1 - \frac{\sqrt{S_1S_3}}{S_2})\right] + \frac{1}{2}(1 + \sqrt{\frac{S_3}{S_1S_2}}) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$

$\tilde{a}_{32} = \frac{\sqrt{210}}{2}\frac{S_3}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$

$\tilde{a}_{33} = -\sqrt{70}\frac{S_3}{\sqrt{S_3}}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[\frac{9}{2} + \sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$

$\tilde{a}_{34} = \frac{3}{2}\sqrt{70}\frac{S_3}{\sqrt{S_4}}aaaa + \cdots$

$\tilde{a}_{35} = -\frac{3}{2}\sqrt{14}\sqrt{S_5}\,aaaaa + \cdots$

$\tilde{a}_{60} = S_6\left[1 - \frac{21}{S_1}a^+a + \frac{105}{S_2}a^+a^+aa + \cdots\right]$

$\tilde{a}_{61} = -\sqrt{21}\frac{S_6}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[10 + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[10\left[3 - (\frac{S_1}{S_2}) + \frac{1}{\sqrt{S_2}}(1 - \frac{\sqrt{S_1S_3}}{S_2})\right] + \frac{1}{2}(1 + \sqrt{\frac{S_3}{S_1S_2}}) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$

$\tilde{a}_{62} = \sqrt{105}\frac{S_6}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$

$\tilde{a}_{63} = -\sqrt{315}\frac{S_6}{\sqrt{S_3}}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[\frac{15}{4} + \sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$

$\tilde{a}_{64} = \frac{15}{4}\sqrt{15}\frac{S_6}{\sqrt{S_4}}aaaa + \cdots$

$\tilde{a}_{65} = -\frac{3}{4}\sqrt{195}\frac{S_6}{\sqrt{S_5}}aaaaa + \cdots$

$\tilde{a}_{66} = \cdots$

$\tilde{a}_{70} = S_7\left[1 - \frac{28}{S_1}a^+a + \frac{189}{S_2}a^+a^+aa + \cdots\right]$

$\tilde{a}_{71} = -\sqrt{28}\frac{S_7}{\sqrt{S_1}}\left[a - \frac{1}{\sqrt{S_2}}\left[\frac{27}{2} + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{27}{2}\left[\frac{25}{6}(\frac{S_1}{S_2}) + \frac{1}{\sqrt{S_2}}(1 - \frac{\sqrt{S_1S_3}}{S_2})\right] + \frac{1}{2}(1 + \sqrt{\frac{S_3}{S_1S_2}}) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$

$\tilde{a}_{72} = 3\sqrt{21}\frac{S_7}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[\frac{25}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$

$\tilde{a}_{73} = -5\sqrt{21}\frac{S_7}{\sqrt{S_3}}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[\frac{11}{2} + \sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$

$\tilde{a}_{74} = \frac{3}{4}\sqrt{462}\frac{S_7}{\sqrt{S_4}}aaaa + \cdots$

$\tilde{a}_{75} = -\frac{3}{2}\sqrt{231}\frac{S_7}{\sqrt{S_5}}aaaaa + \cdots$

$\tilde{a}_{76} = \cdots$

$\tilde{a}_{77} = \cdots$

$$\tilde{Q}_{80} = S_8\left[1 - \frac{36}{S_1}a^+a + \frac{315}{S_2}a^+a^+aa \cdots\right]$$

$$\tilde{Q}_{81} = -\sqrt{36}\,\frac{S_8}{\sqrt{S_1}}\left[a - \left[\frac{35}{2} + \sqrt{S_2} - \frac{S_2}{S_1}\right]a^+aa + \left[\frac{35}{2}\left[\frac{11}{2}\left(\frac{S_1}{S_2}\right) + \frac{1}{\sqrt{S_2}}\left(1 - \frac{\sqrt{S_1S_3}}{S_2}\right)\right] + \frac{1}{2}\left(1 + \sqrt{\frac{S_3}{S_1S_2}}\right) - \frac{\sqrt{S_2}}{S_1}\right]a^+a^+aaa + \cdots\right]$$

$$\tilde{Q}_{82} = 3\sqrt{55}\,\frac{S_8}{\sqrt{S_2}}\left[aa - \sqrt{\frac{S_2}{S_1S_3}}\left[11 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right]a^+aaa + \cdots\right]$$

$$\tilde{Q}_{83} = -\sqrt{1155}\,\frac{S_8}{\sqrt{S_3}}\left[aaa - \sqrt{\frac{S_3}{S_1S_4}}\left[\frac{15}{2} + \sqrt{\frac{S_1S_4}{S_3}} - \frac{S_4}{S_3}\right]a^+aaaa + \cdots\right]$$

$$\tilde{Q}_{84} = \frac{15}{4}\sqrt{195}\,\frac{S_8}{\sqrt{S_4}}aaaa + \cdots$$

$$\tilde{Q}_{85} = -\frac{3}{2}\sqrt{1001}\,\frac{S_8}{\sqrt{S_5}}aaaaa + \cdots$$

$$\tilde{Q}_{86} = \cdots$$

$$\tilde{Q}_{87} = \cdots$$

$$\tilde{Q}_{88} = \cdots$$

Table 5

Stevens operator equivalents expanded in Bose operators

$$S_n = J(J-\tfrac{1}{2})(J-1)\ldots(J-\tfrac{n-1}{2})$$

$$O_2^0(e) = 2\,\tilde{O}_{20} \qquad = 2S_2\left\{1 - \frac{2}{S_1}a^+a + \frac{1}{2S_2}a^+a^+aa\right\}$$

$$O_2^2(e) = \frac{2}{\sqrt{6}}\frac{1}{\sqrt{2}}(\tilde{O}_{2,-2} + \tilde{O}_{2,2}) \qquad = \sqrt{S_2}\left\{(a^+a^+ + aa) - \sqrt{\frac{S_2}{S_1S_3}}\left[\sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right](a^+a^+a^+a + a^+aaa) + \cdots\right\}$$

$$O_4^0(e) = 8\,\tilde{O}_{40} \qquad = 8S_4\left\{1 - \frac{10}{S_1}a^+a + \frac{45}{2S_2}a^+a^+aa \cdots\right\}$$

$$O_4^2(e) = \frac{4}{\sqrt{5}}\frac{1}{\sqrt{2}}(\tilde{O}_{4,-2} + \tilde{O}_{4,2}) \qquad = 6\frac{S_4}{\sqrt{S_2}}\left\{(a^+a^+ + aa) - \sqrt{\frac{S_2}{S_1S_3}}\left[\frac{7}{3} + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right](a^+a^+a^+a + a^+aaa) + \cdots\right\}$$

$$O_4^4(e) = \frac{8}{\sqrt{35}}\frac{1}{\sqrt{2}}(\tilde{O}_{4,-4} + \tilde{O}_{4,4}) \qquad = 2\sqrt{S_4}\,(a^+a^+a^+a^+ + aaaa) + \cdots$$

$$O_6^0(e) = 16\,\tilde{O}_{60} \qquad = 16S_6\left\{1 - \frac{21}{S_1}a^+a + \frac{105}{S_2}a^+a^+aa + \cdots\right\}$$

$$O_6^2(e) = \frac{32}{\sqrt{210}}\frac{1}{\sqrt{2}}(\tilde{O}_{6,-2} + \tilde{O}_{6,2}) \qquad = 16\frac{S_6}{\sqrt{S_2}}\left\{(a^+a^+ + aa) - \sqrt{\frac{S_2}{S_1S_3}}\left[6 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right](a^+a^+a^+a + a^+aaa) + \cdots\right\}$$

$$O_6^4(e) = \frac{16}{3\sqrt{7}}\frac{1}{\sqrt{2}}(\tilde{O}_{6,-4} + \tilde{O}_{6,4}) \qquad = 20\frac{S_6}{\sqrt{S_4}}(a^+a^+a^+a^+ + aaaa) + \cdots$$

$$O_6^6(e) = \cdots$$

$$O_8^0(e) = 128\,\tilde{O}_{80} \qquad = 128\,S_8\left\{1 - \frac{36}{S_1}a^+a + \frac{315}{S_2}a^+a^+aa + \cdots\right\}$$

$$O_8^2(e) = \frac{64}{3\sqrt{70}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-2} + \tilde{O}_{8,2}) \qquad = 32\frac{S_8}{\sqrt{S_2}}\left\{(a^+a^+ + aa) - \sqrt{\frac{S_2}{S_1S_3}}\left[11 + \sqrt{\frac{S_1S_3}{S_2}} - \frac{S_3}{S_2}\right](a^+a^+a^+a + a^+aaa) + \cdots\right\}$$

$$O_8^4(e) = \frac{64}{3\sqrt{7}}\frac{1}{\sqrt{2}}(\tilde{O}_{8,-4} + \tilde{O}_{8,4}) \qquad = 80\frac{S_8}{\sqrt{S_4}}(a^+a^+a^+a^+ + aaaa) + \cdots$$

$$O_8^6(e) = \cdots$$

$$O_8^8(e) = \cdots$$

Table 6

Rotated stevens operators

$$O_2^0(c) \rightsquigarrow \frac{1}{2}\left(3\cos^2\beta-1\right) O_2^0(c) - \frac{3}{2}\sin^2\beta\, O_2^2(c)$$
$$+ 3\sin\beta\cos\beta\, O_2^1(s)$$

$$O_2^2(c) \rightsquigarrow \left\{\frac{1}{2}\sin^2\beta\, O_2^0(c) - \frac{1}{2}\left(1+\cos^2\beta\right) O_2^2(c) - 2\sin\beta\cos\beta\, O_2^1(s)\right\}\cos 2\alpha$$

$$O_4^0(c) \rightsquigarrow \frac{1}{8}\left(35\cos^4\beta-30\cos^2\beta+3\right) O_4^0(c) + \frac{35}{8}\sin^4\beta\, O_4^4(c)$$
$$-\frac{5}{2}\sin^2\beta\left(7\cos^2\beta-1\right) O_4^2(c) - 35\cos\beta\sin^3\beta\, O_4^3(s)$$
$$+5\sin\beta\cos\beta\left(7\cos^2\beta-3\right) O_4^1(s)$$

$$O_4^2(c) \rightsquigarrow \left\{\frac{1}{8}\sin^2\beta\left(7\cos^2\beta-1\right) O_4^0(c) + \frac{7}{8}\sin^2\beta\left(1+\cos^2\beta\right) O_4^4(c)\right.$$
$$-\frac{1}{8}\left[1+15\sin^4\beta-12\sin^2\beta\left(1+\cos^2\beta\right)+\cos^4\beta+6\cos^2\beta\right] O_4^2(c)$$
$$\left.-7\sin\beta\cos^3\beta\, O_4^3(s) + \sin\beta\cos\beta\left(4-7\cos^2\beta\right) O_4^1(s)\right\}\cos 2\alpha$$
$$+\left\{-\frac{7}{4}\sin^2\beta\cos\beta\, O_4^4(s) - \frac{1}{8}\left[24\sin^2\beta-4\left(1+\cos^2\beta\right)\right]\cos\beta\, O_4^2(s)\right.$$
$$\left.+\frac{7}{2}\sin\beta\left(1-3\cos^2\beta\right) O_4^3(c) + \frac{1}{2}\left(1-7\sin\beta\cos^2\beta\right) O_4^1(c)\right\}\sin 2\alpha$$

$$
\begin{aligned}
O_4^4(c) \rightsquigarrow \Big\{ & \tfrac{1}{8}\sin^4\beta\, O_4^0(c) + \left[\tfrac{1}{8} + \tfrac{3}{4}\cos^2\beta + \tfrac{1}{8}\cos^4\beta\right] O_4^4(c) \\
& - \tfrac{1}{2}\sin^2\beta\,(1+\cos^2\beta)\, O_4^2(c) + \sin\beta\,(\cos^3\beta + 3\cos\beta)\, O_4^3(s) \\
& - \sin^3\beta\cos\beta\, O_4^1(s) \Big\} \cos 4\alpha \\
+ \Big\{ & -\tfrac{1}{2}\cos\beta\,(1+\cos^2\beta)\, O_4^4(s) + \sin^2\beta\cos\beta\, O_4^2(s) \\
& + \sin\beta\,(1+3\cos^2\beta)\, O_4^3(c) - \sin^3\beta\, O_4^1(c) \Big\} \sin 4\alpha
\end{aligned}
$$

$$
\begin{aligned}
O_6^0(c) \rightsquigarrow\ & \tfrac{1}{16}\left(231\cos^6\beta - 315\cos^4\beta + 105\cos^2\beta - 5\right) O_6^0(c) \\
& - \tfrac{105}{32}\left(33\cos^4\beta - 18\cos^2\beta + 1\right)\sin^2\beta\, O_6^2(c) \\
& + \tfrac{63}{16}\left(11\cos^2\beta - 1\right)\sin^4\beta\, O_6^4(c) - \tfrac{231}{32}\sin^6\beta\, O_6^6(c) \\
& + \tfrac{21}{4}\left(33\cos^5\beta - 30\cos^3\beta + 5\cos\beta\right)\sin\beta\, O_6^1(s) \\
& - \tfrac{105}{8}\left(11\cos^3\beta - 3\cos\beta\right)\sin^3\beta\, O_6^3(s) + \tfrac{231}{8}\cos\beta\sin^5\beta\, O_6^5(s)
\end{aligned}
$$

$$
\begin{aligned}
O_6^2(c) \rightsquigarrow \Big\{ & \tfrac{1}{16} \sin^2\beta \,(33\cos^4\beta - 18\cos^2\beta + 1)\, O_6^0(c) \\
& - \tfrac{1}{32} \left[495\cos^6\beta - 735\cos^4\beta + 289\cos^2\beta - 17 \right] O_6^2(c) \\
& + \tfrac{3}{16} \sin^2\beta \,(33\cos^4\beta - 10\cos^2\beta + 1)\, O_6^4(c) \\
& - \tfrac{33}{32} \sin^4\beta \,(1 + \cos^2\beta)\, O_6^6(c) + \tfrac{33}{8} \sin^3\beta \,(\cos\beta + 3\cos^3\beta)\, O_6^5(s) \\
& - \tfrac{3}{8} \sin\beta \,(11\cos\beta - 50\cos^3\beta + 55\cos^5\beta)\, O_6^3(s) \\
& + \tfrac{1}{4} \sin\beta \,(-18\cos\beta + 102\cos^3\beta - 99\cos^5\beta)\, O_6^1(s) \Big\} \cos 2\alpha \\
+ \Big\{ & \tfrac{1}{32} (74\cos\beta - 372\cos^3\beta + 330\cos^5\beta)\, O_6^2(s) \\
& + \tfrac{3}{16} \sin^2\beta \,(20\cos\beta - 44\cos^3\beta)\, O_6^4(s) \\
& + \tfrac{33}{16} \sin^4\beta \cos\beta \, O_6^6(s) - \tfrac{33}{8} \sin^3\beta \,(1 - 5\cos^2\beta)\, O_6^5(c) \\
& + \tfrac{3}{8} \sin\beta \,(-3 + 42\cos^2\beta - 55\cos^4\beta)\, O_6^3(c) \\
& - \tfrac{1}{4} \sin\beta \,(1 - 18\cos^2\beta + 33\cos^4\beta)\, O_6^1(c) \Big\} \sin 2\alpha
\end{aligned}
$$

$$
\begin{aligned}
O_6^4(c) \rightsquigarrow \Big\{ & \tfrac{1}{16} \sin^4\beta\,(11\cos^2\beta - 1)\, O_6^0(c) \\
& - \tfrac{11}{32} \sin^2\beta\,(1 + 6\cos^2\beta + \cos^4\beta)\, O_6^6(c) \\
& + \tfrac{1}{16}\,(13 - 65\cos^2\beta + 35\cos^4\beta + 33\cos^6\beta)\, O_6^4(c) \\
& - \tfrac{5}{32} \sin^2\beta\,(1 - 10\cos^2\beta + 33\cos^4\beta)\, O_6^2(c) \\
& + \tfrac{11}{8} \sin\beta\,(-5\cos\beta + 10\cos^3\beta + 3\cos^5\beta)\, O_6^5(s) \\
& - \tfrac{5}{8}\,(5\cos\beta - 2\cos^3\beta - 11\cos^5\beta)\, O_6^3(s) \\
& + \tfrac{1}{4} \sin^3\beta\,(13\cos\beta - 33\cos^3\beta)\, O_6^1(s) \Big\} \cos 4\alpha \\
+ \Big\{ & \tfrac{11}{32} \sin^2\beta\,(4\cos\beta + 4\cos^3\beta)\, O_6^6(s) \\
& + \tfrac{1}{16}\,(-8\cos\beta + 80\cos^3\beta - 88\cos^5\beta)\, O_6^4(s) \\
& - \tfrac{5}{32} \sin^2\beta\,(20\cos\beta - 44\cos^3\beta)\, O_6^2(s) \\
& - \tfrac{11}{8} \sin\beta\,(2 - 10\cos^4\beta)\, O_6^5(c) \\
& + \tfrac{5}{8} \sin\beta\,(2 - 16\cos^2\beta + 22\cos^4\beta)\, O_6^3(c) \\
& + \tfrac{1}{4} \sin^3\beta\,(2 - 22\cos^2\beta)\, O_6^1(s) \Big\} \sin 4\alpha
\end{aligned}
$$

$$
\begin{aligned}
O_6^6(c) \rightsquigarrow \Big\{ & \tfrac{1}{16}\sin^6\beta\, O_6^0(c) - \tfrac{15}{32}\sin^4\beta\,(1+\cos^2\beta)\, O_6^2(c) \\
& + \tfrac{3}{16}\sin^2\beta\,(1+6\cos^2\beta+\cos^4\beta)\, O_6^4(c) \\
& - \tfrac{1}{32}(1+15\cos^2\beta+15\cos^4\beta+\cos^6\beta)\, O_6^6(c) \\
& - \tfrac{3}{8}\sin\beta\,(\cos^5\beta+10\cos^3\beta+5\cos\beta)\, O_6^5(s) \\
& + \tfrac{5}{8}\sin^3\beta\,(\cos^3\beta+3\cos\beta)\, O_6^3(s) - \tfrac{3}{4}\sin^5\beta\cos\beta\, O_6^1(s) \Big\} \cos 6\alpha \\
+ \Big\{ & \tfrac{1}{32}(3\cos\beta+10\cos^3\beta+3\cos^5\beta)\, O_6^6(s) \\
& - \tfrac{3}{4}\sin^2\beta(\cos\beta+\cos^3\beta)\, O_6^4(s) + \tfrac{15}{16}\sin^4\beta\cos\beta\, O_6^2(s) \\
& - \tfrac{3}{8}\sin\beta\,(1+10\cos^2\beta+5\cos^4\beta)\, O_6^5(c) \\
& + \tfrac{5}{8}\sin^3\beta\,(1+3\cos^2\beta)\, O_6^3(c) - \tfrac{3}{4}\sin^5\beta\, O_6^1(c) \Big\} \sin 6\alpha
\end{aligned}
$$

Table 7

Differentiated, rotated Stevens operators

$$\frac{\partial}{\partial\beta}\langle O_2^0(c)\rangle = -\frac{3}{2}\left(\langle O_2^0(c)\rangle + \langle O_2^2(c)\rangle\right)\sin 2\beta$$

$$\frac{\partial}{\partial\beta}\langle O_2^2(c)\rangle = \frac{1}{2}\left(\langle O_2^0(c)\rangle + \langle O_2^2(c)\rangle\right)\cos 2\alpha\,\sin 2\beta$$

$$\begin{aligned}\frac{\partial}{\partial\beta}\langle O_4^0(c)\rangle = &-5\left(\langle O_4^0(c)\rangle + 3\langle O_4^2(c)\rangle\right)\sin 2\beta\\ &+\frac{35}{4}\left(\langle O_4^0(c)\rangle + 4\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\right)\sin^2\beta\,\sin 2\beta\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial\beta}\langle O_4^2(c)\rangle = &\frac{1}{4}\left(3\langle O_4^0(c)\rangle + 16\langle O_4^2(c)\rangle + 7\langle O_4^4(c)\rangle\right)\cos 2\alpha\,\sin 2\beta\\ &-\frac{7}{4}\left(\langle O_4^0(c)\rangle + 4\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\right)\cos 2\alpha\,\sin^2\beta\,\sin 2\beta\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial\beta}\langle O_4^4(c)\rangle = &-\left(\frac{1}{2}\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\right)\cos 4\alpha\,\sin 2\beta\\ &+\frac{1}{4}\left(\langle O_4^0(c)\rangle + 4\langle O_4^2(c)\rangle + \langle O_4^4(c)\rangle\right)\cos 4\alpha\,\sin^2\beta\,\sin 2\beta\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial\beta}\langle O_6^0(c)\rangle = &-\frac{21}{2}\left(\langle O_6^0(c)\rangle + 5\langle O_6^2(c)\rangle\right)\sin 2\beta\\ &+\frac{189}{4}\left(\langle O_6^0(c)\rangle + \frac{20}{3}\langle O_6^2(c)\rangle + \frac{5}{3}\langle O_6^4(c)\rangle\right)\sin^2\beta\,\sin 2\beta\\ &-\frac{693}{16}\left(\langle O_6^0(c)\rangle + \frac{15}{2}\langle O_6^2(c)\rangle + 3\langle O_6^4(c)\rangle + \frac{1}{2}\langle O_6^6(c)\rangle\right)\sin^4\beta\,\sin 2\beta\end{aligned}$$

$$\frac{\partial}{\partial\beta}\langle O_6^2(c)\rangle = \left(\langle O_6^0(c)\rangle + \frac{19}{2}\langle O_6^2(c)\rangle + \frac{9}{2}\langle O_6^4(c)\rangle\right)\cos 2\alpha \sin 2\beta$$

$$-6\left(\langle O_6^0(c)\rangle + \frac{125}{16}\langle O_6^2(c)\rangle + \frac{3}{2}\langle O_6^4(c)\rangle + \frac{11}{16}\langle O_6^6(c)\rangle\right)\cos 2\alpha \sin^2\beta \sin 2\beta$$

$$+\frac{99}{16}\left(\langle O_6^0(c)\rangle + \frac{15}{2}\langle O_6^2(c)\rangle + 3\langle O_6^4(c)\rangle + \frac{1}{2}\langle O_6^6(c)\rangle\right)\cos 2\alpha \sin^4\beta \sin 2\beta$$

$$\frac{\partial}{\partial\beta}\langle O_6^4(c)\rangle = -\left(\frac{15}{4}\langle O_6^2(c)\rangle + \frac{13}{2}\langle O_6^4(c)\rangle + \frac{11}{16}\langle O_6^6(c)\rangle\right)\cos 4\alpha \sin 2\beta$$

$$+\left(\frac{5}{4}\langle O_6^0(c)\rangle + \frac{25}{2}\langle O_6^2(c)\rangle + \frac{67}{4}\langle O_6^4(c)\rangle + \frac{11}{2}\langle O_6^6(c)\rangle\right)\cos 4\alpha \sin^2\beta \sin 2\beta$$

$$-\left(\frac{33}{16}\langle O_6^0(c)\rangle + \frac{495}{32}\langle O_6^2(c)\rangle + \frac{99}{16}\langle O_6^4(c)\rangle + \frac{33}{32}\langle O_6^6(c)\rangle\right)\cos 4\alpha \sin^4\beta \sin 2\beta$$

$$\frac{\partial}{\partial\beta}\langle O_6^6(c)\rangle = \left(\frac{3}{2}\langle O_6^4(c)\rangle + \frac{3}{2}\langle O_6^6(c)\rangle\right)\cos 6\alpha \sin 2\beta$$

$$-\left(\frac{15}{8}\langle O_6^2(c)\rangle + 3\langle O_6^4(c)\rangle\right) - \frac{9}{8}\langle O_6^6(c)\rangle\Big)\cos 6\alpha \sin^2\beta \sin 2\beta$$

$$+\left(\frac{3}{16}\langle O_6^0(c)\rangle + \frac{45}{32}\langle O_6^2(c)\rangle + \frac{9}{16}\langle O_6^4(c)\rangle + \frac{3}{32}\langle O_6^6(c)\rangle\right)\cos 6\alpha \sin^4\beta \sin 2\beta$$

$$\frac{\partial}{\partial\alpha}\langle O_6^6(c)\rangle = \Big\{\left(\frac{1}{16}\langle O_6^0(c)\rangle + \frac{15}{32}\langle O_6^2(c)\rangle + \frac{3}{16}\langle O_6^4(c)\rangle + \frac{1}{32}\langle O_6^6(c)\rangle\right)\sin^6\beta$$

$$+\left(-\frac{15}{16}\langle O_6^2(c)\rangle - \frac{3}{2}\langle O_6^4(c)\rangle - \frac{9}{16}\langle O_6^6(c)\rangle\right)\sin^4\beta$$

$$+\left(\frac{3}{2}\langle O_6^4(c)\rangle + \frac{3}{2}\langle O_6^6(c)\rangle\right)\sin^2\beta - \langle O_6^6(c)\rangle\Big\}(-6\sin 6\alpha$$

Table 8

Fourier transforms of Bose operatorexpressions

$$a_l = \frac{1}{\sqrt{N}} \sum_q e^{-i\bar{q}\cdot\bar{R}_l} a_q \quad \curvearrowleft \quad a_q = \frac{1}{\sqrt{N}} \sum_l e^{i\bar{q}\cdot\bar{R}_l} a_l$$

$$a_l^{\dagger} = \frac{1}{\sqrt{N}} \sum_q e^{i\bar{q}\cdot\bar{R}_l} a_q^{\dagger} \quad \curvearrowleft \quad a_q^{\dagger} = \frac{1}{\sqrt{N}} \sum_l e^{-i\bar{q}\cdot\bar{R}_l} a_l^{\dagger}$$

$$J(\bar{R}_{ll'}) = \frac{1}{N} \sum_q J(\bar{q})\, e^{-i\bar{q}\cdot\bar{R}_{ll'}} \curvearrowleft J(\bar{q}) = \sum_{R_{ll'}} J(\bar{R}_{ll'})\, e^{i\bar{q}\cdot\bar{R}_{ll'}}$$

$$J(\bar{R}_{lm}) = \frac{1}{N} \sum_q J'(\bar{q})\, e^{-i\bar{q}\cdot\bar{R}_{lm}} \curvearrowleft J'(\bar{q}) = \sum_{R_{lm}} J(\bar{R}_{lm})\, e^{i\bar{q}\cdot\bar{R}_{lm}}$$

$$\sum_q e^{i\bar{q}\cdot(\bar{R}_l - \bar{R}_{l'})} = N\delta_{ll'}$$

$$\sum_{l>l'} e^{i(\bar{q}-\bar{q}')\cdot(\bar{R}_l - \bar{R}_{l'})} = \frac{1}{2} N\delta_{qq'}$$

$$\sum_{l,l'} e^{i(\bar{q}-\bar{q}')\cdot(\bar{R}_l - \bar{R}_{l'})} = N\delta_{qq'}$$

$$\sum_{\ell} a_\ell^\dagger a_\ell = \sum_{q} a_q^\dagger a_q$$

$$\sum_{\ell} a_\ell a_\ell = \sum_{q} a_q a_{-q}$$

$$\sum_{\ell} a_\ell^\dagger a_\ell^\dagger = \sum_{q} a_q^\dagger a_{-q}^\dagger$$

$$\sum_{\ell,\ell'} a_\ell^\dagger a_{\ell'} = \sum_{\substack{q \\ \bar{R}_{\ell\ell'}}} e^{i\bar{q}\cdot\bar{R}_{\ell\ell'}} a_q^\dagger a_q$$

$$\sum_{\ell,\ell'} a_\ell a_{\ell'} = \sum_{\substack{q \\ \bar{R}_{\ell\ell'}}} e^{i\bar{q}\bar{R}_{\ell\ell'}} a_q a_{-q}$$

$$\sum_{\ell,\ell'} a_\ell^\dagger a_{\ell'}^\dagger = \sum_{\substack{q \\ \bar{R}_{\ell\ell'}}} e^{i\bar{q}\cdot\bar{R}_{\ell\ell'}} a_q^\dagger a_{-q}^\dagger$$

$$\sum_{\ell} a_\ell^\dagger a_\ell^\dagger a_\ell^\dagger a_\ell^\dagger = \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^\dagger a_{q_2}^\dagger a_{-q_3}^\dagger a_{-q_4}^\dagger \, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell} a_\ell^\dagger a_\ell^\dagger a_\ell^\dagger a_\ell = \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^\dagger a_{q_2}^\dagger a_{-q_3}^\dagger a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell} a_\ell^\dagger a_\ell^\dagger a_\ell a_\ell = \frac{1}{N} \sum_{\substack{q_1, q_2 \\ q_3 q_4}} a_{q_1}^\dagger a_{q_2}^\dagger a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell} a_\ell^\dagger a_\ell a_\ell a_\ell = \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{q_1}^\dagger a_{-q_2}^\dagger a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell} a_\ell a_\ell a_\ell a_\ell = \frac{1}{N} \sum_{\substack{q_1 q_2 \\ q_3 q_4}} a_{-q_1} a_{-q_2} a_{q_3} a_{q_4} \, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell>\ell'} \mathcal{J}(\bar{R}_{\ell\ell'})\, a_\ell^\dagger a_\ell = \frac{1}{2}\sum_q \mathcal{J}(0)\, a_q^\dagger a_q$$

$$\sum_{\ell>\ell'} \mathcal{J}(\bar{R}_{\ell\ell'})\, a_\ell^\dagger a_{\ell'} = \frac{1}{2}\sum_q \mathcal{J}(\bar{q})\, a_q^\dagger a_q$$

$$\sum_{m>m'} \mathcal{J}(\bar{R}_{mm'})\, b_m^\dagger b_m = \frac{1}{2}\sum_q \mathcal{J}(0)\, b_q^\dagger b_q$$

$$\sum_{m>m'} \mathcal{J}(\bar{R}_{mm'})\, b_m^\dagger b_{m'} = \frac{1}{2}\sum_q \mathcal{J}(\bar{q})\, b_q^\dagger b_q$$

$$\sum_{\ell,m} \mathcal{J}(\bar{R}_{\ell m})\, a_\ell^\dagger a_\ell = \sum_q \mathcal{J}'(0)\, a_q^\dagger a_q$$

$$\sum_{\ell,m} \mathcal{J}(\bar{R}_{\ell m})\, b_m^\dagger b_m = \sum_q \mathcal{J}'(0)\, b_q^\dagger b_q$$

$$\sum_{\ell,m} \mathcal{J}(\bar{R}_{\ell,m})\, a_\ell^\dagger b_m = \sum_q \mathcal{J}'(\bar{q})\, a_q^\dagger b_q$$

$$\sum_{\ell,m} \mathcal{J}(\bar{R}_{\ell,m})\, a_\ell b_m^\dagger = \sum_q \mathcal{J}'(\bar{q})^*\, a_q b_q^\dagger$$

$$\sum_{\ell>\ell'} J(\bar{R}_{\ell\ell'})\, a_\ell^+ a_\ell a_{\ell'}^+ a_{\ell'} = \frac{1}{2N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J(\bar{q}_4 - \bar{q}_2)\, a_{q_1}^+ a_{q_2}^+ a_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell>\ell'} J(\bar{R}_{\ell\ell'})\, a_\ell^+ a_{\ell'}^+ a_{\ell'} a_\ell = \frac{1}{2N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J(\bar{q}_4)\, a_{q_1}^+ a_{q_2}^+ a_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell>\ell'} J(\bar{R}_{\ell\ell'})\, a_\ell^+ a_{\ell'}^+ a_{\ell'} a_{\ell'} = \frac{1}{2N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J(\bar{q}_1)\, a_{q_1}^+ a_{q_2}^+ a_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell,m} J(\bar{R}_{\ell m})\, a_\ell^+ b_m^+ a_\ell b_m = \frac{1}{N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J'(\bar{q}_4 - \bar{q}_2)\, a_{q_1}^+ b_{q_2}^+ a_{q_3} b_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell,m} J(\bar{R}_{\ell m})\, a_\ell^+ a_\ell^+ a_\ell b_m = \frac{1}{N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J'(\bar{q}_4)\, a_{q_1}^+ a_{q_2}^+ a_{q_3} b_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell,m} J(\bar{R}_{\ell m})\, b_m^+ b_m^+ b_m a_\ell = \frac{1}{N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J'(\bar{q}_4)^* b_{q_1}^+ b_{q_2}^+ b_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell,m} J(\bar{R}_{\ell m})\, a_\ell^+ b_m^+ a_\ell a_\ell = \frac{1}{N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J'(\bar{q}_2)^* a_{q_1}^+ b_{q_2}^+ a_{q_3} a_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

$$\sum_{\ell,m} J(\bar{R}_{\ell m})\, b_m^+ a_\ell^+ b_m b_m = \frac{1}{N} \sum_{\substack{q_1 q_2\\ q_3 q_4}} J'(\bar{q}_2)\, b_{q_1}^+ a_{q_2}^+ b_{q_3} b_{q_4}\, \delta_{q_1+q_2,\, q_3+q_4}$$

Table 9

Two magnon interactions treated in the Hartree-Fock approximation

$$\mathcal{H}_1 = \frac{D_1}{N} \sum_{\substack{K_1K_2\\K_3K_4}} a^\dagger_{K_1} a^\dagger_{K_2} a_3 a_4 \, \delta_{K_1+K_2,\,K_3+K_4}$$

$$\Delta E_0(1) = -2D_1 \sum_{K_1} \langle a^\dagger_{K_1} a_{K_1} \rangle$$
$$- \frac{D_1}{N} \sum_{K_1K_2} \left(2\langle a^\dagger_{K_1} a_{K_1} \rangle \langle a^\dagger_{K_2} a_{K_2} \rangle + \langle a^\dagger_{K_1} a^\dagger_{-K_1} \rangle \langle a_{K_2} a_{-K_2} \rangle \right)$$

$$\Delta A_K(1) = \frac{4D_1}{N} \sum_{K_1} \langle a^\dagger_{K_1} a_{K_1} \rangle$$

$$\Delta B_K(1) = \frac{2D_1}{N} \sum_{K_1} \langle a^\dagger_{K_1} a_{-K_1} \rangle$$

$$\mathcal{H}_2 = \frac{D_2}{N} \sum_{\substack{K_1K_2\\K_3K_4}} \left(a^\dagger_{K_1} a^\dagger_{K_2} a^\dagger_{-K_3} a_{K_4} + a^\dagger_{K_1} a_{-K_2} a_{K_3} a_{K_4} \right) \delta_{K_1+K_2,\,K_3+K_4}$$

$$\Delta E_0(2) = -\frac{3}{2} D_2 \sum_{K_1} \left(\langle a^\dagger_{K_1} a^\dagger_{-K_1} \rangle + \langle a_{K_1} a_{-K_1} \rangle \right)$$
$$- \frac{3D_2}{N} \sum_{K_1K_2} \langle a^\dagger_{K_2} a_{K_2} \rangle \left(\langle a^\dagger_{K_1} a^\dagger_{-K_1} \rangle + \langle a_{K_1} a_{-K_1} \rangle \right)$$

$$\Delta A_K(2) = \frac{3D_2}{N} \sum_{K_1} \left(\langle a^\dagger_{K_1} a^\dagger_{-K_1} \rangle + \langle a_{K_1} a_{-K_1} \rangle \right)$$

$$\Delta B_K(2) = \frac{6D_2}{N} \sum_{K_1} \langle a^\dagger_{K_1} a_{K_1} \rangle$$

$$\mathcal{H}_3 = \frac{D_3}{N} \sum_{\substack{K_1 K_2 \\ K_3 K_4}} \left(a^{+}_{K_1} a^{+}_{K_2} a^{+}_{-K_3} a^{+}_{-K_4} + a_{-K_1} a_{-K_2} a_{K_3} a_{K_4} \right) \delta_{K_1+K_2,\, K_3+K_4}$$

$$\Delta E_0(3) = -\frac{3D_3}{N} \sum_{K_1 K_2} \left(\langle a^{+}_{K_1} a^{+}_{-K_1} \rangle \langle a^{+}_{K_2} a^{+}_{-K_2} \rangle + \langle a_{K_1} a_{-K_1} \rangle \langle a_{K_2} a_{-K_2} \rangle \right)$$

$$\Delta A_K(3) = 0$$

$$\Delta B_K(3) = \frac{12 D_3}{N} \sum_{K_1} \langle a_{K_1} a_{-K_1} \rangle$$

$$\mathcal{H}_4 = \frac{D_4}{N} \sum_{\substack{K_1 K_2 \\ K_3 K_4}} \mathcal{J}'(\underline{K}_4 - \underline{K}_2)\, a^{+}_{K_1} b^{+}_{K_2} a_{K_3} b_{K_4}\, \delta_{K_1+K_2,\, K_3+K_4}$$

$$\Delta E_0(4) = -\frac{D_4}{2} \sum_{K_1} \mathcal{J}'(0) \left(\langle a^{+}_{K_1} a_{K_1} \rangle + \langle b^{+}_{K_1} b_{K_1} \rangle \right)$$

$$- \frac{D_4}{N} \sum_{K_1 K_2} \mathcal{J}'(\underline{K}_1 - \underline{K}_2) \left(\langle a^{+}_{K_1} b_{K_1} \rangle \langle b^{+}_{K_2} a_{K_2} \rangle + \langle a^{+}_{K_1} b^{+}_{-K_1} \rangle \langle a_{K_2} b_{-K_2} \rangle \right)$$

$$- \frac{D_4}{N} \sum_{K_1 K_2} \mathcal{J}'(0) \langle a^{+}_{K_1} a_{K_1} \rangle \langle b^{+}_{K_2} b_{K_2} \rangle$$

$$\Delta A^{a}_{K}(4) = \frac{D_4}{N} \sum_{K_2} \mathcal{J}'(0) \langle b^{+}_{K_2} b_{K_2} \rangle$$

$$\Delta A^{b}_{K}(4) = \frac{D_4}{N} \sum_{K_2} \mathcal{J}'(0) \langle a^{+}_{K_2} a_{K_2} \rangle$$

$$\Delta B^{a}_{K}(4) = 0$$

$$\Delta B^{b}_{K}(4) = 0$$

$$\Delta C_K(4) = \frac{D_4}{N}\sum_{K_1} \mathcal{F}'(\underline{K}_1-\underline{K}_2)\langle a^{+}_{K_1} b_{K_1}\rangle$$

$$\Delta C_K(4)^{*} = \frac{D_4}{N}\sum_{K_1} \mathcal{F}'(\underline{K}_1-\underline{K}_2)^{*}\langle b^{+}_{K_1} a_{K_1}\rangle$$

$$\Delta D_K(4) = \frac{D_4}{N}\sum_{K_1} \mathcal{F}'(\underline{K}_1-\underline{K}_2)\langle a^{+}_{K_1} b^{+}_{-K_1}\rangle$$

$$\Delta D_K(4)^{*} = \frac{D_4}{N}\sum_{K_1} \mathcal{F}'(\underline{K}_1-\underline{K}_2)\langle a_{K_1} b_{-K_1}\rangle$$

$$\mathcal{H}_5 = \frac{D_5}{N}\sum_{\substack{K_1K_2\\K_3K_4}} \mathcal{F}'(\underline{K}_2)\, b^{+}_{K_1} a^{+}_{K_2} b_{K_3} b_{K_4}\, \delta_{K_1+K_2,K_3+K_4}$$

$$\Delta E_0(5) = -D_5\sum_{K_1} \mathcal{F}'(\underline{K}_2)\langle a^{+}_{K_1} b_{K_1}\rangle$$

$$-\frac{D_5}{N}\sum_{K_1K_2} \mathcal{F}'(\underline{K}_2)\Big(2\langle b^{+}_{K_1} b_{K_1}\rangle\langle a^{+}_{K_2} b_{K_2}\rangle + \langle b^{+}_{-K_2} a^{+}_{K_2}\rangle\langle b_{K_1} b_{-K_1}\rangle\Big)$$

$$\Delta A^{a}_K(5) = 0$$

$$\Delta A^{b}_K(5) = \frac{D_5}{N}\sum_{K_2} 2\mathcal{F}'(\underline{K}_2)\langle a^{+}_{K_2} b_{K_2}\rangle$$

$$\Delta B^{a}_K(5) = 0$$

$$\Delta B^{a}_K(5)^{*} = 0$$

$$\Delta B^{b}_K(5) = \frac{D_5}{N}\sum_{K_2} 2\mathcal{F}'(\underline{K}_2)\langle b^{+}_{-K_2} a^{+}_{K_2}\rangle$$

$$\Delta B^{b}_K(5)^{*} = 0$$

$$\Delta C_K(5) = 0$$

$$\Delta C_K(5)^* = \frac{D_5}{N} \sum_{K_1} 2 \mathcal{F}'(\underline{K}_2) \langle b^{+}_{K_1} b_{K_1} \rangle$$

$$\Delta D_K(5) = 0$$

$$\Delta D_K(5)^* = \frac{D_5}{N} \sum_{K_1} \mathcal{F}'(\underline{K}_2) \langle b_{K_1} b_{-K_1} \rangle$$

$$\mathcal{H}_6 = \frac{D_6}{N} \sum_{\substack{K_1 K_2 \\ K_3 K_4}} \mathcal{F}'(\underline{K}_2)^* a^{+}_{K_1} b^{+}_{K_2} a_{K_3} a_{K_4} \delta_{K_1+K_2,\, K_3+K_4}$$

$$\Delta E_0(6) = -D_6 \sum_{K_2} \mathcal{F}'(\underline{K}_2)^* \langle b^{+}_{K_2} a_{K_2} \rangle$$

$$- \frac{D_6}{N} \sum_{K_1 K_2} \mathcal{F}'(\underline{K}_2)^* \Big(2 \langle a^{+}_{K_1} a_{K_1} \rangle \langle b^{+}_{K_2} a_{K_2} \rangle + \langle a^{+}_{K_2} b^{+}_{-K_2} \rangle \langle a_{K_1} a_{-K_1} \rangle \Big)$$

$$\Delta A^a_K(6) = \frac{D_6}{N} \sum_{K_2} 2 \mathcal{F}'(\underline{K}_2)^* \langle b^{+}_{K_2} a_{K_2} \rangle$$

$$\Delta A^b_K(6) = 0$$

$$\Delta B^a_K(6) = \frac{D_6}{N} \sum_{K_2} 2 \mathcal{F}'(\underline{K}_2)^* \langle a^{+}_{K_2} b^{+}_{-K_2} \rangle$$

$$\Delta B^a_K(6)^* = 0$$

$$\Delta B^b_K(6) = 0$$

$$\Delta B^b_K(6)^* = 0$$

$$\Delta C_K(6) = \frac{D_6}{N} \sum_{K_1} 2 \mathcal{J}'(\underline{K}_2)^* \langle a^+_{K_1} a_{K_1} \rangle$$

$$\Delta C_K(6)^* = 0$$

$$\Delta D_K(6) = 0$$

$$\Delta D_K(6)^* = \frac{D_6}{N} \sum_{K_1} \mathcal{J}'(\underline{K}_2)^* \langle a_{K_1} a_{-K_1} \rangle$$

$$\mathcal{H}_7 = \frac{D_7}{N} \sum_{\substack{K_1 K_2 \\ K_3 K_4}} \mathcal{J}'(\underline{K}_4)\, a^+_{K_1} a^+_{K_2} a_{K_3} b_{K_4} \quad \delta_{K_1+K_2,\, K_3+K_4}$$

$$\Delta E_0(7) = - D_7 \sum_{K_2} \mathcal{J}'(\underline{K}_2) \langle a^+_{K_2} b_{K_2} \rangle$$
$$- \frac{D_7}{N} \sum_{K_1 K_2} \Big(2 \mathcal{J}'(\underline{K}_2) \langle a^+_{K_1} a_{K_1} \rangle \langle a^+_{K_2} b_{K_2} \rangle +$$
$$\mathcal{J}'(\underline{K}_2)^* \langle a^+_{-K_1} a^+_{K_1} \rangle \langle a^+_{K_2} b_{-K_2} \rangle \Big)$$

$$\Delta A^a_K(7) = \frac{D_7}{N} \sum_{K_2} 2 \mathcal{J}'(\underline{K}_2) \langle a^+_{K_2} b_{K_2} \rangle$$

$$\Delta A^b_K(7) = 0$$

$$\Delta B^a_K(7) = 0$$

$$\Delta B^a_K(7)^* = \frac{D_7}{N} \sum_{K_2} 2 \mathcal{J}'(\underline{K}_2)^* \langle a_{K_2} b_{-K_2} \rangle$$

$$\Delta B^b_K(7) = 0$$

$$\Delta B^b_K(7)^* = 0$$

$$\Delta C_K(7) = 0$$

$$\Delta C_K(7)^* = \frac{D_7}{N} \sum_{K_1} 2\,\mathcal{J}'(\underline{K}_2) \langle a^+_{K_1} a_{K_1} \rangle$$

$$\Delta D_K(7) = \frac{D_7}{N} \sum_{K_1} \mathcal{J}'(\underline{K}_2)^* \langle a^+_{-K_1} a^+_{K_1} \rangle$$

$$\Delta D_K(7)^* = 0$$

$$\mathcal{H}_8 = \frac{D_8}{N} \sum_{\substack{K_1K_2\\K_3K_4}} \mathcal{J}'(\underline{K}_4)^* b^+_{K_1} b^+_{K_2} b_{K_3} a_{K_4} \delta_{K_1+K_2, K_3+K_4}$$

$$\Delta E_0(8) = -D_8 \sum_{K_2} \mathcal{J}'(\underline{K}_2)^* \langle b^+_{K_2} a_{K_2} \rangle$$

$$- \frac{D_8}{N} \sum_{K_1K_2} \Big(2\,\mathcal{J}'(\underline{K}_2)^* \langle b^+_{K_1} b_{K_1} \rangle \langle b^+_{K_2} a_{K_2} \rangle$$

$$+ \mathcal{J}'(\underline{K}_2)^* \langle b^+_{-K_1} b^+_{K_1} \rangle \langle b_{-K_2} a_{K_2} \rangle \Big)$$

$$\Delta A^a_K(8) = 0$$

$$\Delta A^b_K(8) = \frac{D_8}{N} \sum_{K_2} 2\,\mathcal{J}'(\underline{K}_2)^* \langle b^+_{K_2} a_{K_2} \rangle$$

$$\Delta B^a_K(8) = 0$$

$$\Delta B^a_K(8)^* = 0$$

$$\Delta B^b_K(8) = 0$$

$$\Delta B^b_K(8)^* = \frac{D_8}{N} \sum_{K_2} 2\,\mathcal{J}'(\underline{K}_2)^* \langle b_{-K_2} a_{K_2} \rangle$$

$$\Delta C_K(8) = \frac{D_8}{N}\sum_{K_1} 2\,\mathcal{J}'(\underline{K}_2)^* \langle b^+_{K_1} b_{K_1}\rangle$$

$$\Delta C_K(8)^* = 0$$

$$\Delta D_K(8) = \frac{D_8}{N}\sum_{K_1} \mathcal{J}'(\underline{K}_2)^* \langle b^+_{-K_1} b^+_{K_1}\rangle$$

$$\Delta D_K(8)^* = 0$$

$$\mathcal{H}_9 = \frac{D_9}{2N}\sum_{\substack{K_1K_2\\K_3K_4}}\Big(2(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_4)+\mathcal{J}(\underline{K}_1)\big) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big)\times$$
$$\times\, a^+_{K_1} a^+_{K_2} a_{K_3} a_{K_4}\, \delta_{K_1+K_2,\,K_3+K_4}$$

$$\Delta E_0(9) = -\frac{D_9}{2N}\sum_{K_1}\Big\{4(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big) - \mathcal{J}(0)$$
$$- \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}\langle a^+_{K_1} a_{K_1}\rangle$$
$$- \frac{D_9}{2N}\sum_{K_1K_2}\Big\{2(S_1-\sqrt{S_2})\big(3\,\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big) - \mathcal{J}(0)$$
$$- \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}\langle a^+_{K_1} a_{K_1}\rangle\langle a^+_{K_2} a_{K_2}\rangle$$
$$- \frac{D_9}{2N}\sum_{K_1K_2}\Big\{2(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}$$
$$\times\langle a^+_{K_1} a^+_{-K_1}\rangle\langle a_{K_2} a_{-K_2}\rangle$$

$$\Delta A^a_K(9) = \frac{D_9}{N}\sum_{K_2}\Big\{4(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big) - \mathcal{J}(0)$$
$$- \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}\langle a^+_{K_2} a_{K_2}\rangle$$

$$\Delta B^a_K(9) = \frac{D_9}{N}\sum_{K_1}\Big\{2(S_1-\sqrt{S_2})\big(\mathcal{J}(\underline{K}_1)+\mathcal{J}(\underline{K}_2)\big) - \mathcal{J}(\underline{K}_1-\underline{K}_2)\Big\}$$
$$\times\langle a^+_{K_1} a^+_{-K_1}\rangle$$

Table 10

Correlation functions of Racah operators

$$\langle O_2^1(s)\,O_2^1(s)\rangle = -\frac{1}{6}\left\{5\begin{Bmatrix}2&2&2\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_2\|J\rangle\left[\frac{1}{2}\,\frac{1}{\sqrt{2\cdot5\cdot7}}\langle O_2^0(c)\rangle-\sqrt{\frac{3}{5\cdot7}}\,\frac{2}{\sqrt{6}}\langle O_2^2(c)\rangle\right]\right.$$

$$\left.+9\begin{Bmatrix}2&2&4\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_2\|J\rangle)^2}{\langle J\|\tilde{O}_4\|J\rangle}\left[\frac{1}{8}\sqrt{\frac{2^5}{3^2\cdot5\cdot7}}\langle O_4^0(c)\rangle-\sqrt{\frac{2^2}{3^2\cdot7}}\,\frac{4}{\sqrt{10}}\langle O_4^2(c)\rangle\right]\right\}$$

$$\langle O_4^1(s)\,O_4^1(s)\rangle = -\frac{4}{5}\left\{5\begin{Bmatrix}4&4&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\left[\frac{17}{3}\sqrt{\frac{1}{5\cdot7\cdot11}}\,\frac{1}{2}\langle O_2^0(c)\rangle-\sqrt{\frac{2\cdot5}{3\cdot7\cdot11}}\,\frac{2}{\sqrt{6}}\langle O_2^2(c)\rangle\right]\right.$$

$$+9\begin{Bmatrix}4&4&4\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_4\|J\rangle\left[-6\sqrt{\frac{1}{2\cdot7\cdot11\cdot13}}\,\frac{1}{8}\langle O_4^0(c)\rangle+18\sqrt{\frac{5}{7\cdot11\cdot13}}\,\frac{4}{\sqrt{10}}\langle O_4^2(c)\rangle\right]$$

$$\left.+13\begin{Bmatrix}4&4&6\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_6\|J\rangle}\left[-\frac{1}{3}\sqrt{\frac{1}{5\cdot11\cdot13}}\,\frac{1}{16}\langle O_6^0(c)\rangle-\sqrt{\frac{7}{3\cdot11\cdot13}}\,\frac{16}{\sqrt{105}}\langle O_6^2(c)\rangle\right]\right\}$$

$$\langle O_4^3(s)\,O_4^3(s)\rangle = -\frac{4}{35}\left\{-10\begin{Bmatrix}4&4&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\,\frac{1}{2}\sqrt{\frac{7}{2^2\cdot3^2\cdot5\cdot11}}\langle O_2^0(c)\rangle\right.$$

$$+18\begin{Bmatrix}4&4&4\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_4\|J\rangle\,\frac{1}{8}\sqrt{\frac{7}{2\cdot11\cdot13}}\langle O_4^0(c)\rangle$$

$$\left.+26\begin{Bmatrix}4&4&6\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_6\|J\rangle}\,\frac{1}{16}\sqrt{\frac{2^2}{3^2\cdot5\cdot11\cdot13}}\langle O_6^0(c)\rangle\right\}$$

$$\Big(\langle O_4^3(s)\,O_4^1(s)\rangle+\langle O_4^1(s)\,O_4^3(s)\rangle\Big)=-\frac{4}{5\sqrt{7}}\Bigg\{-10\begin{Bmatrix}4&4&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\frac{2}{\sqrt{6}}\sqrt{\frac{3}{2\cdot5\cdot11}}\,\langle O_2^2(c)\rangle$$

$$-18\begin{Bmatrix}4&4&4\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_4\|J\rangle\left[\sqrt{\frac{5}{3^2\cdot11\cdot13}}\frac{4}{\sqrt{70}}\langle O_4^2(c)\rangle+\sqrt{\frac{5\cdot7}{3^2\cdot11\cdot13}}\frac{8}{\sqrt{70}}\langle O_4^4(c)\rangle\right]$$

$$+26\begin{Bmatrix}4&4&6\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_4\|J\rangle)^2}{\langle J\|\tilde{O}_6\|J\rangle}\left[\sqrt{\frac{3}{11\cdot13}}\frac{16}{\sqrt{105}}\langle O_6^2(c)\rangle+\sqrt{\frac{7}{2\cdot5\cdot11\cdot13}}\frac{16}{3\sqrt{14}}\langle O_6^4(c)\rangle\right]\Bigg\}$$

$$\langle O_6^1(s)\,O_6^1(s)\rangle=-\frac{32}{21}\Bigg\{5\begin{Bmatrix}6&6&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\left[\frac{2}{\sqrt{2\cdot5\cdot7\cdot11\cdot13}}\frac{1}{2}\langle O_2^0(c)\rangle-\sqrt{\frac{3\cdot7}{5\cdot11\cdot13}}\frac{2}{\sqrt{6}}\langle O_2^2(c)\rangle\right]$$

$$+9\begin{Bmatrix}6&6&4\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_4\|J\rangle}\left[\frac{-2}{\sqrt{3^2\cdot7\cdot11\cdot13\cdot17}}\frac{1}{8}\langle O_4^0(c)\rangle+\sqrt{\frac{2^3\cdot5\cdot7}{3^2\cdot11\cdot13\cdot17}}\frac{4}{\sqrt{10}}\langle O_4^2(c)\rangle\right]$$

$$+13\begin{Bmatrix}6&6&6\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_6\|J\rangle\left[\frac{-2}{\sqrt{2\cdot3\cdot7\cdot13}}\frac{1}{16}\langle O_6^0(c)\rangle-\sqrt{\frac{2^2\cdot3\cdot5\cdot7}{11\cdot13\cdot17\cdot19}}\frac{16}{\sqrt{105}}\langle O_6^2(c)\rangle\right]\Bigg\}$$

$$\langle O_6^1(c)\, O_6^1(c)\rangle = \frac{32}{21}\Bigg\{ 5 \begin{Bmatrix} 6 & 6 & 2 \\ J & J & J \end{Bmatrix} \frac{(\langle J \| \tilde{O}_6 \| J\rangle)^2}{\langle J \| \tilde{O}_2 \| J\rangle} \left[\frac{-2}{\sqrt{2\cdot 5\cdot 7\cdot 11\cdot 13}}\, \frac{1}{2} \langle O_2^0(c)\rangle - \sqrt{\frac{3\cdot 7}{5\cdot 11\cdot 13}}\, \frac{2}{\sqrt{6}} \langle O_2^2(c)\rangle \right]$$

$$+ 9 \begin{Bmatrix} 6 & 6 & 4 \\ J & J & J \end{Bmatrix} \frac{(\langle J \| \tilde{O}_6 \| J\rangle)^2}{\langle J \| \tilde{O}_4 \| J\rangle} \left[\frac{2}{\sqrt{3^2\cdot 7\cdot 11\cdot 13\cdot 17}}\, \frac{1}{8} \langle O_4^0(c)\rangle + \sqrt{\frac{2^3\cdot 5\cdot 7}{3^2\cdot 11\cdot 13\cdot 17}}\, \frac{4}{\sqrt{10}} \langle O_4^2(c)\rangle \right]$$

$$+ 13 \begin{Bmatrix} 6 & 6 & 6 \\ J & J & J \end{Bmatrix} \langle J \| \tilde{O}_6 \| J\rangle \left[\frac{2}{\sqrt{2\cdot 3\cdot 7\cdot 13}}\, \frac{1}{16} \langle O_6^0(c)\rangle - \sqrt{\frac{2^2\cdot 3\cdot 5\cdot 7}{11\cdot 13\cdot 17\cdot 19}}\, \frac{16}{\sqrt{105}} \langle O_6^2(c)\rangle \right] \Bigg\}$$

$$\langle O_6^3(s)\, O_6^3(s)\rangle = \langle O_6^3(c)\, O_6^3(c)\rangle \cong -\frac{64}{105} \Bigg\{ 10 \begin{Bmatrix} 6 & 6 & 2 \\ J & J & J \end{Bmatrix} \frac{(\langle J \| \tilde{O}_6 \| J\rangle)^2}{\langle J \| \tilde{O}_2 \| J\rangle}\, \frac{1}{2} \sqrt{\frac{5}{2\cdot 7\cdot 11\cdot 13}}\, \langle O_2^0(c)\rangle$$

$$+ 18 \begin{Bmatrix} 6 & 6 & 4 \\ J & J & J \end{Bmatrix} \frac{(\langle J \| \tilde{O}_6 \| J\rangle)^2}{\langle J \| \tilde{O}_4 \| J\rangle}\, \frac{1}{8} \sqrt{\frac{3\cdot 7}{11\cdot 13\cdot 17}}\, \langle O_4^0(c)\rangle$$

$$- 26 \begin{Bmatrix} 6 & 6 & 6 \\ J & J & J \end{Bmatrix} \langle J \| \tilde{O}_6 \| J\rangle\, \frac{1}{16} \sqrt{\frac{2^2}{11\cdot 13\cdot 17\cdot 19}}\, \langle O_6^0(c)\rangle \Bigg\}$$

$$\langle O_6^3(c)\, O_6^3(s)\rangle = i\,\frac{64}{105}\left\{-6\begin{Bmatrix}6&6&1\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_1\|J\rangle}\sqrt{\frac{3}{2\cdot 7\cdot 13}}\,\langle O_1^0(c)\rangle\right.$$

$$+14\begin{Bmatrix}6&6&3\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_3\|J\rangle}\,\frac{1}{2}\sqrt{\frac{2^4}{7\cdot 11\cdot 13}}\,\langle O_3^0(c)\rangle$$

$$\left.-22\begin{Bmatrix}6&6&5\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_5\|J\rangle}\,\frac{1}{8}\sqrt{\frac{11}{2^2\cdot 7\cdot 13\cdot 17}}\,\frac{1}{8}\langle O_5^0(c)\rangle\right\}$$

$$\langle O_6^5(s)\, O_6^5(s)\rangle = \langle O_6^5(c)\, O_6^5(c)\rangle \cong -\frac{64}{693}\left\{-10\begin{Bmatrix}6&6&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\,\frac{1}{2}\sqrt{\frac{11}{2\cdot 5\cdot 7\cdot 13}}\,\langle O_2^0(c)\rangle\right.$$

$$+18\begin{Bmatrix}6&6&4\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_4\|J\rangle}\,\frac{1}{8}\sqrt{\frac{11}{7\cdot 13\cdot 17}}\,\langle O_4^0(c)\rangle$$

$$\left.+26\begin{Bmatrix}6&6&6\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_6\|J\rangle\,\frac{1}{16}\sqrt{\frac{5^2\cdot 11}{2^2\cdot 13\cdot 17\cdot 19}}\,\langle O_6^0(c)\rangle\right\}$$

$$\langle O_6^5(c)\, O_6^5(s)\rangle = i\,\frac{64}{693}\left\{-6\begin{Bmatrix}6&6&1\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_1\|J\rangle}\sqrt{\frac{5^2}{2\cdot 3\cdot 7\cdot 13}}\,\langle O_1^0(c)\rangle\right.$$

$$\left.+22\begin{Bmatrix}6&6&5\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_5\|J\rangle}\sqrt{\frac{3^2\cdot 11}{2^2\cdot 7\cdot 13\cdot 17}}\,\frac{1}{8}\langle O_5^0(c)\rangle\right\}$$

$$\left(\langle O_6^1(s)\,O_6^3(s)\rangle + \langle O_6^3(s)\,O_6^1(s)\rangle\right) = -\frac{64}{21\sqrt{10}}\Bigg\{-10\begin{Bmatrix}6&6&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\frac{2}{\sqrt{6}}\sqrt{\frac{2^3\cdot 3}{7\cdot 11\cdot 13}}\,\langle O_2^2(c)\rangle$$

$$+18\begin{Bmatrix}6&6&4\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_4\|J\rangle}\left[\sqrt{\frac{2^4}{7\cdot 11\cdot 13\cdot 17}}\frac{4}{\sqrt{10}}\langle O_4^2(c)\rangle - \sqrt{\frac{7^2}{11\cdot 13\cdot 17}}\frac{8}{\sqrt{70}}\langle O_4^4(c)\rangle\right]$$

$$+26\begin{Bmatrix}6&6&6\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_6\|J\rangle\left[\sqrt{\frac{3^3\cdot 7}{2\cdot 11\cdot 13\cdot 17\cdot 19}}\frac{16}{\sqrt{105}}\langle O_6^2(c)\rangle + \sqrt{\frac{5^3\cdot 7}{2^2\cdot 11\cdot 13\cdot 17\cdot 19}}\frac{16}{3\sqrt{14}}\langle O_6^4(c)\rangle\right]\Bigg\}$$

$$\left(\langle O_6^1(c)\,O_6^3(c)\rangle + \langle O_6^3(c)\,O_6^1(c)\rangle\right) = \frac{64}{21\sqrt{10}}\Bigg\{10\begin{Bmatrix}6&6&2\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_2\|J\rangle}\frac{2}{\sqrt{6}}\sqrt{\frac{2^3\cdot 3}{7\cdot 11\cdot 13}}\,\langle O_2^2(c)\rangle$$

$$+18\begin{Bmatrix}6&6&4\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_4\|J\rangle}\left[-\sqrt{\frac{2^4}{7\cdot 11\cdot 13\cdot 17}}\frac{4}{\sqrt{10}}\langle O_4^2(c)\rangle - \sqrt{\frac{7^2}{11\cdot 13\cdot 17}}\frac{8}{\sqrt{70}}\langle O_4^4(c)\rangle\right]$$

$$+26\begin{Bmatrix}6&6&6\\J&J&J\end{Bmatrix}\langle J\|\tilde{O}_6\|J\rangle\left[-\sqrt{\frac{3^3\cdot 7}{2\cdot 11\cdot 13\cdot 17\cdot 19}}\frac{16}{\sqrt{105}}\langle O_6^2(c)\rangle + \sqrt{\frac{5^3\cdot 7}{2^2\cdot 11\cdot 13\cdot 17\cdot 19}}\frac{16}{3\sqrt{14}}\langle O_6^4(c)\rangle\right]\Bigg\}$$

$$\langle O_6^1(c)\,O_6^3(s)\rangle = i\,\frac{64}{21\sqrt{10}}\Bigg\{-7\begin{Bmatrix}6&6&3\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_3\|J\rangle}\sqrt{\frac{2^3\cdot 3}{7\cdot 11\cdot 13}}\frac{2}{\sqrt{30}}\,\langle O_3^2(c)\rangle$$

$$+11\begin{Bmatrix}6&6&5\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_5\|J\rangle}\left[\sqrt{\frac{3^3}{11\cdot 13\cdot 17}}\frac{4}{\sqrt{210}}\langle O_5^2(c)\rangle + \sqrt{\frac{7^2}{2^2\cdot 11\cdot 13\cdot 17}}\frac{8}{3\sqrt{70}}\langle O_5^4(c)\rangle\right]\Bigg\}$$

$$\left(\langle O_6^1(s)\,O_6^5(s)\rangle + \langle O_6^5(s)\,O_6^1(s)\rangle\right) =$$

$$\left(\langle O_6^1(c)\,O_6^5(c)\rangle + \langle O_6^5(c)\,O_6^1(c)\rangle\right) \cong -\frac{64}{21\sqrt{66}}\left\{-18\begin{Bmatrix}6&6&4\\7&7&7\end{Bmatrix}\frac{(\langle 7\|\tilde{O}_6\|7\rangle)^2}{\langle 7\|\tilde{O}_4\|7\rangle}\sqrt{\frac{5}{3\cdot 13\cdot 17}}\,\frac{8}{\sqrt{70}}\,\langle O_4^4(c)\rangle\right.$$

$$\left. -26\begin{Bmatrix}6&6&6\\7&7&7\end{Bmatrix}\langle 7\|\tilde{O}_6\|7\rangle\sqrt{\frac{3^3\cdot 7}{2^2\cdot 13\cdot 17\cdot 19}}\,\frac{16}{3\sqrt{14}}\,\langle O_6^4(c)\rangle\right\}$$

$$\langle O_6^1(c)\,O_6^5(s)\rangle = -11\begin{Bmatrix}6&6&5\\7&7&7\end{Bmatrix}\frac{(\langle 7\|\tilde{O}_6\|7\rangle)^2}{\langle 7\|\tilde{O}_5\|7\rangle}\,\frac{8}{3\sqrt{70}}\sqrt{\frac{3\cdot 5}{2^2\cdot 13\cdot 17}}\,\langle O_4^5(c)\rangle$$

$$\left(\langle O_6^3(s)\,O_6^5(s)\rangle + \langle O_6^5(s)\,O_6^3(s)\rangle\right) =$$

$$\left(\langle O_6^3(c)\,O_6^5(c)\rangle + \langle O_6^5(c)\,O_6^3(c)\rangle\right) \cong -\frac{64}{21\sqrt{165}}\left\{-10\begin{Bmatrix}6&6&2\\7&7&7\end{Bmatrix}\frac{(\langle 7\|\tilde{O}_6\|7\rangle)^2}{\langle 7\|\tilde{O}_2\|7\rangle}\sqrt{\frac{1}{7\cdot 13}}\,\frac{2}{\sqrt{6}}\,\langle O_2^2(c)\rangle\right.$$

$$-18\begin{Bmatrix}6&6&4\\7&7&7\end{Bmatrix}\frac{(\langle 7\|\tilde{O}_6\|7\rangle)^2}{\langle 7\|\tilde{O}_4\|7\rangle}\sqrt{\frac{2^3\cdot 3}{7\cdot 13\cdot 17}}\,\frac{4}{\sqrt{70}}\,\langle O_4^2(c)\rangle$$

$$\left. +26\begin{Bmatrix}6&6&6\\7&7&7\end{Bmatrix}\langle 7\|\tilde{O}_6\|7\rangle\sqrt{\frac{7}{13\cdot 17\cdot 19}}\,\frac{16}{\sqrt{105}}\,\langle O_6^2(c)\rangle\right\}$$

$$\langle O_6^5(c)\,O_6^3(s)\rangle = \langle O_6^3(c)\,O_6^5(s)\rangle = i\,\frac{64}{21\sqrt{165}}\left\{-7\begin{Bmatrix}6&6&3\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_3\|J\rangle}\,\frac{2}{\sqrt{30}}\sqrt{\frac{2}{7\cdot 13}}\,\langle O_3^2(c)\rangle\right.$$

$$\left.-11\begin{Bmatrix}6&6&5\\J&J&J\end{Bmatrix}\frac{(\langle J\|\tilde{O}_6\|J\rangle)^2}{\langle J\|\tilde{O}_5\|J\rangle}\,\frac{4}{\sqrt{210}}\sqrt{\frac{1}{2\cdot 13\cdot 17}}\,\langle O_5^2(c)\rangle\right\}.$$

$$\langle J\|\tilde{O}_1\|J\rangle = \frac{1}{2}\sqrt{\frac{(2J+2)!}{(2J-1)!}}$$

$$\langle J\|\tilde{O}_2\|J\rangle = \frac{1}{4}\sqrt{\frac{(2J+3)!}{(2J-2)!}}$$

$$\langle J\|\tilde{O}_3\|J\rangle = \frac{1}{8}\sqrt{\frac{(2J+4)!}{(2J-3)!}}$$

$$\langle J\|\tilde{O}_4\|J\rangle = \frac{1}{16}\sqrt{\frac{(2J+5)!}{(2J-4)!}}$$

$$\langle J\|\tilde{O}_5\|J\rangle = \frac{1}{32}\sqrt{\frac{(2J+6)!}{(2J-5)!}}$$

$$\langle J\|\tilde{O}_6\|J\rangle = \frac{1}{64}\sqrt{\frac{(2J+7)!}{(2J-6)!}}$$

FIGURES

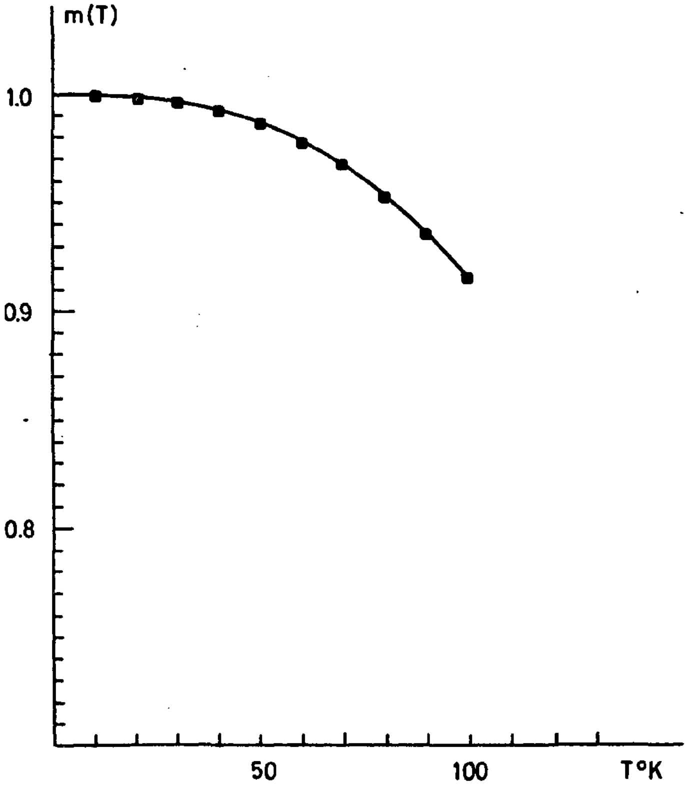

Fig1. THE zero point corrected relative magnetization of Terbium

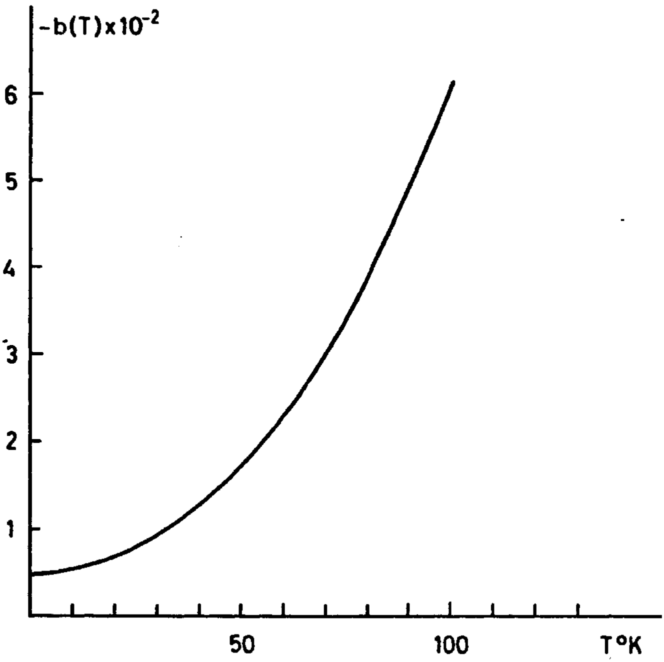

Fig 2. The ellipticity parameter of Terbium

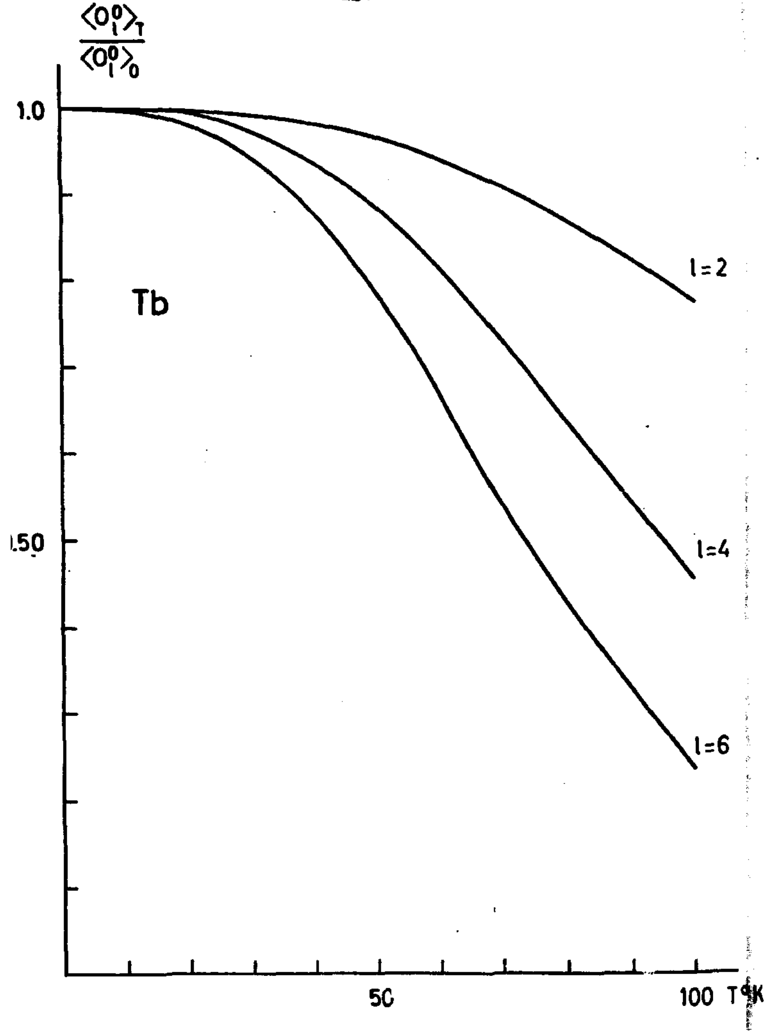

Fig 3. The Stevens Operators

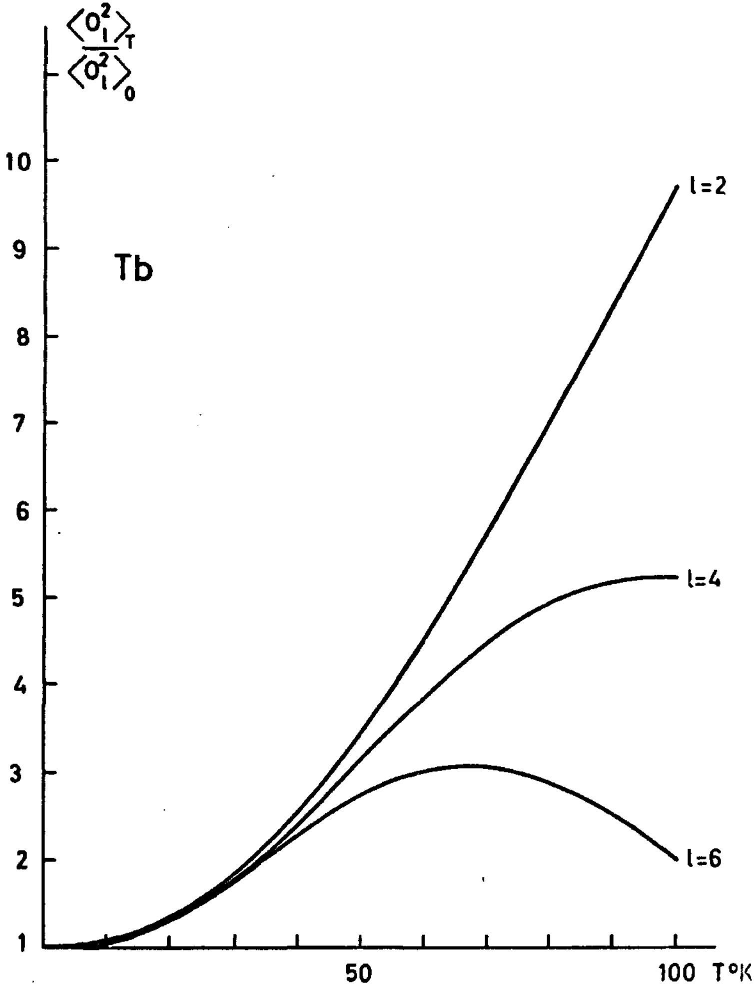

Fig 4. The Stevens Operators

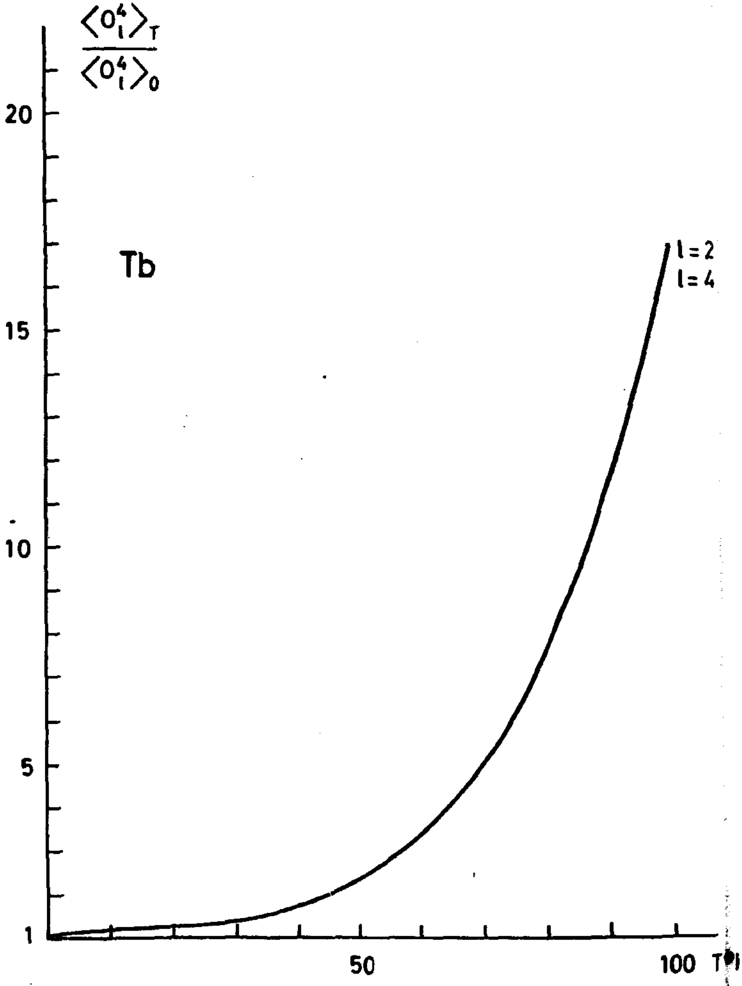

Fig 5. The Stevens Operators

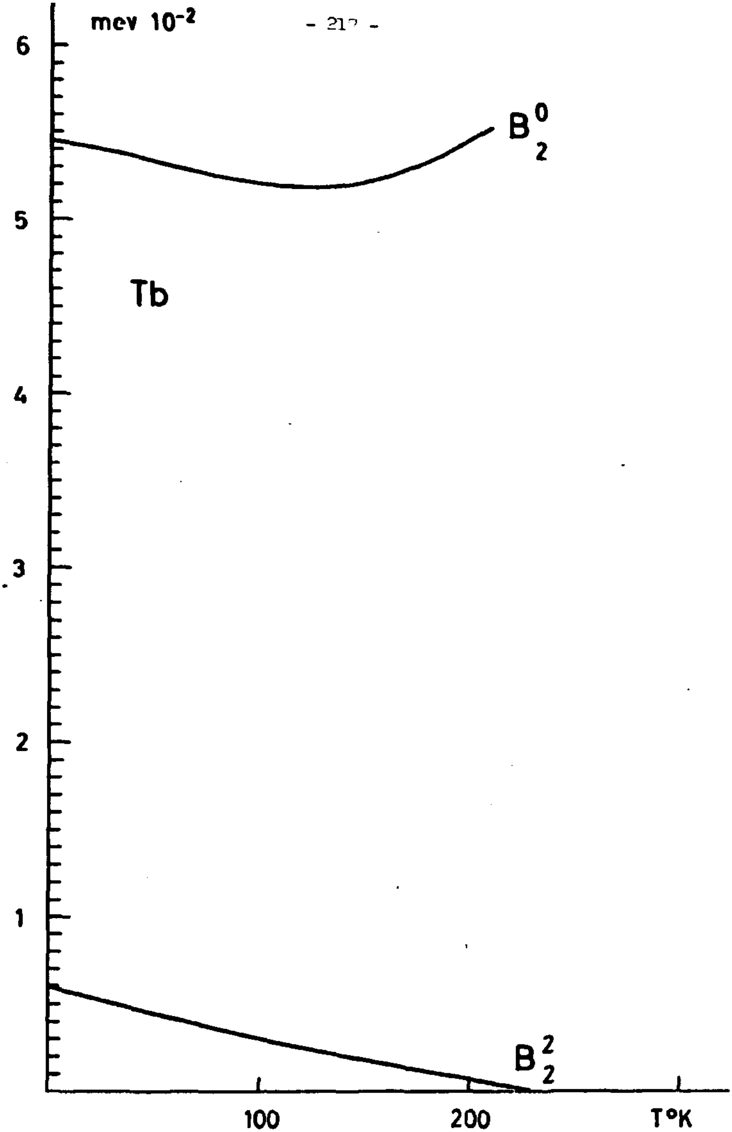

Fig 6. Crystal Field Parameters

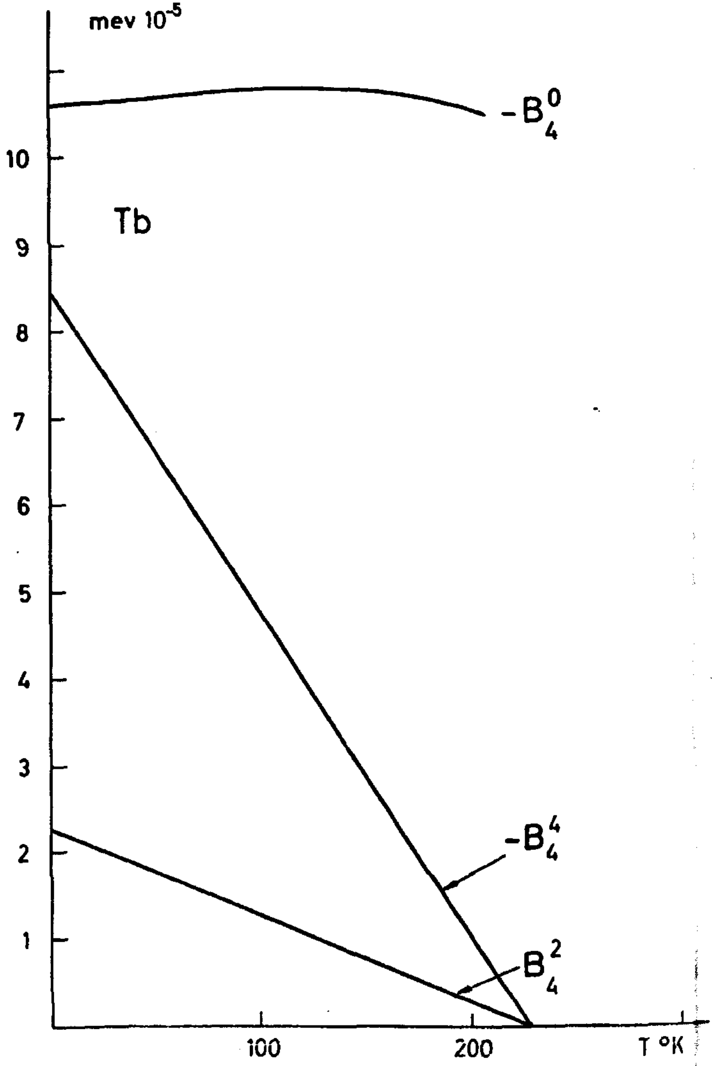

Fig 7. Crystal Field Parameters

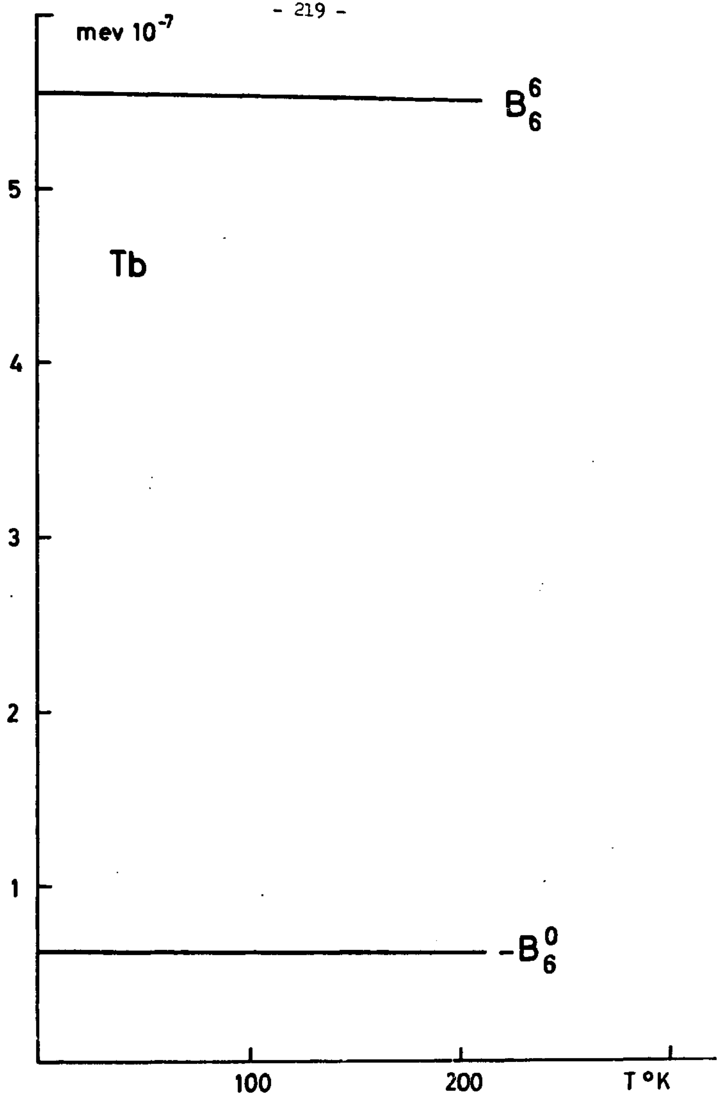

Fig 8. Crystal Field Parameters

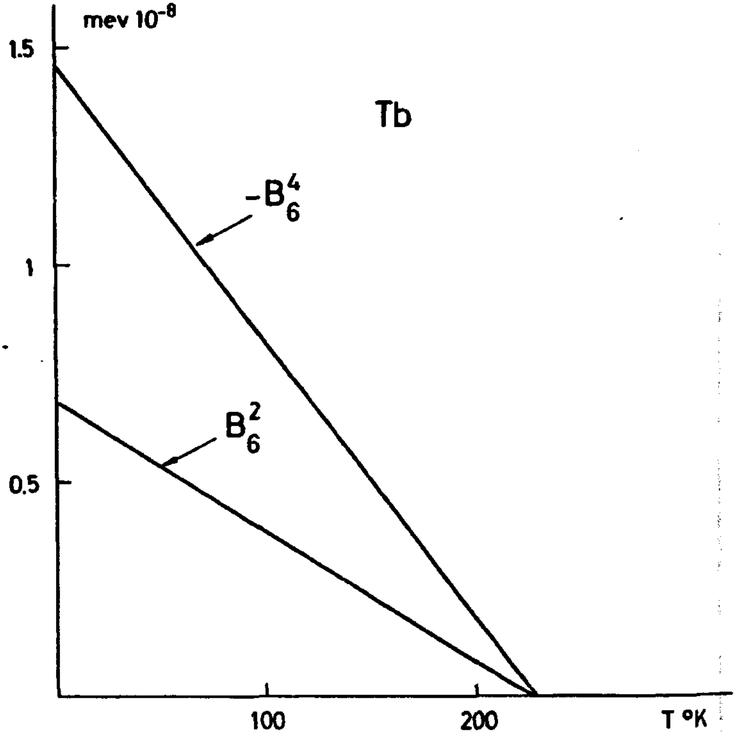

Fig. 9 Crystal Field Parameters

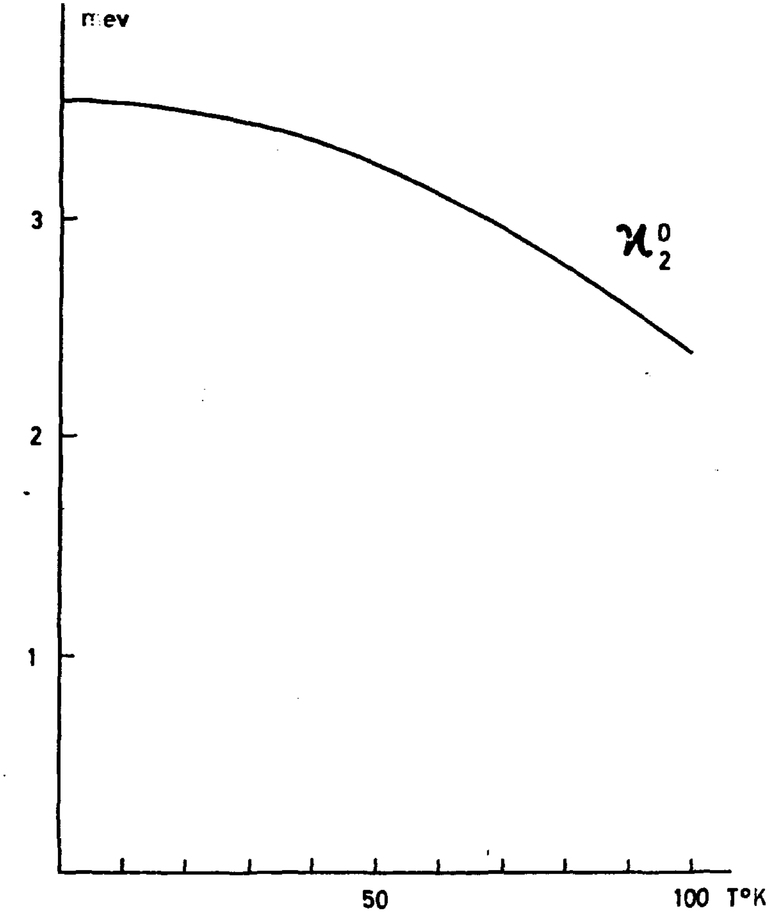

Fig 10. Anisotropy Coefficients of Terbium

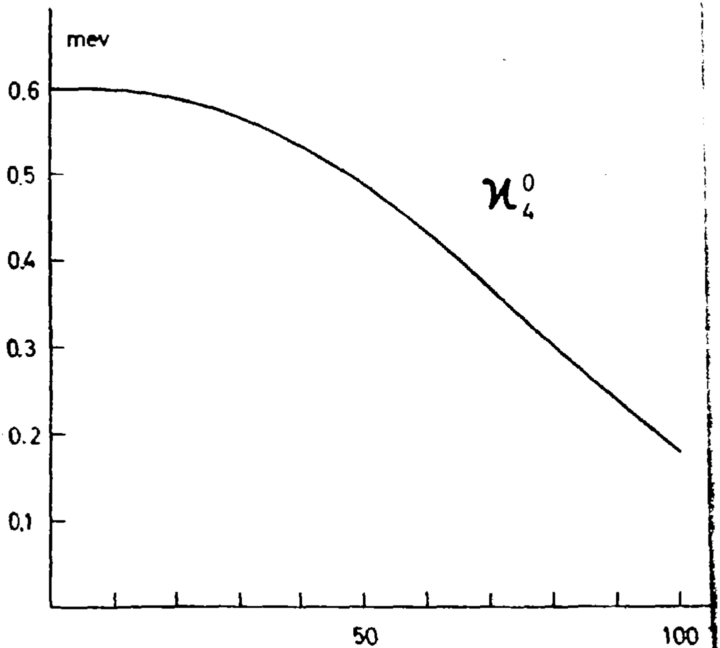

Fig 11. Anisotropy Coefficients of Terbium

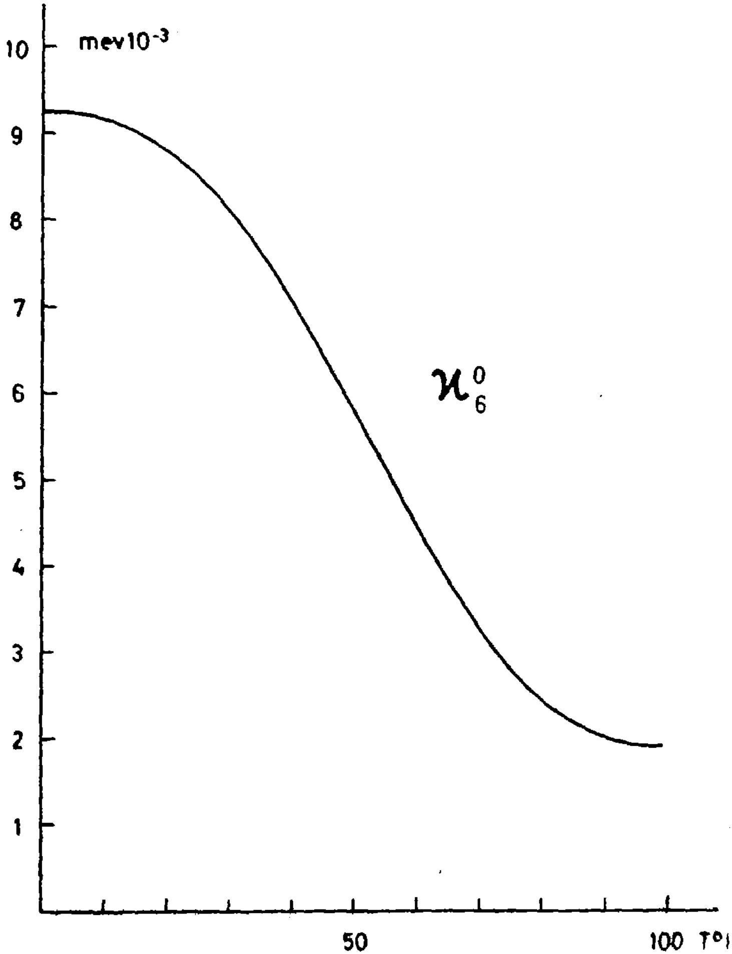

Fig 12. Anisotropy Coefficients of Terbium.

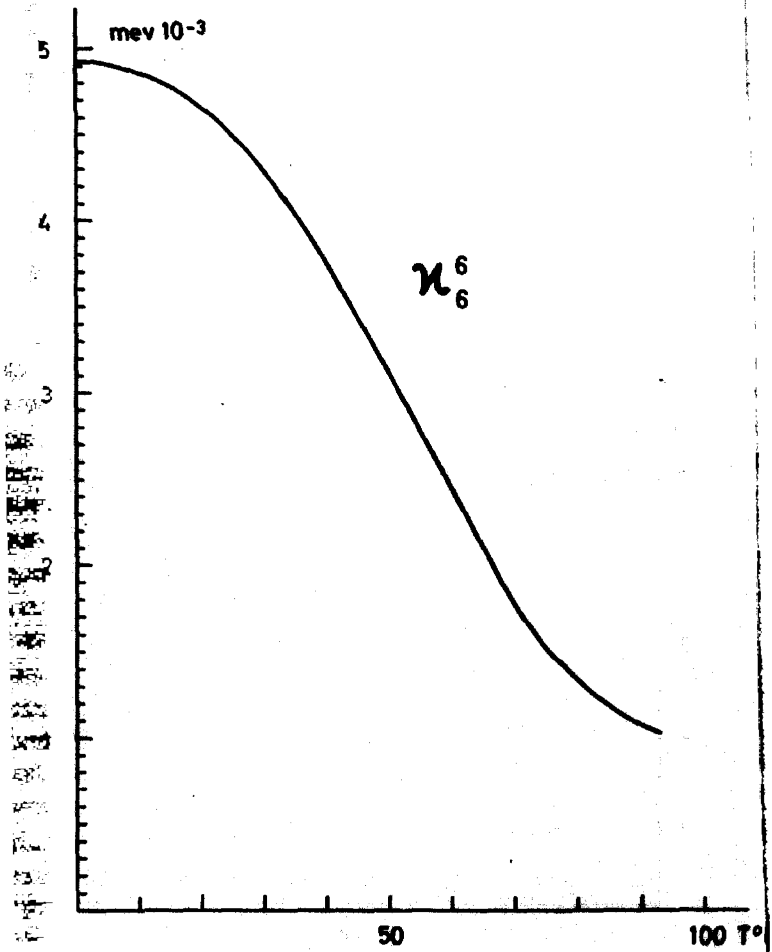

Fig 13. Anisotropy Coefficients of Terbium

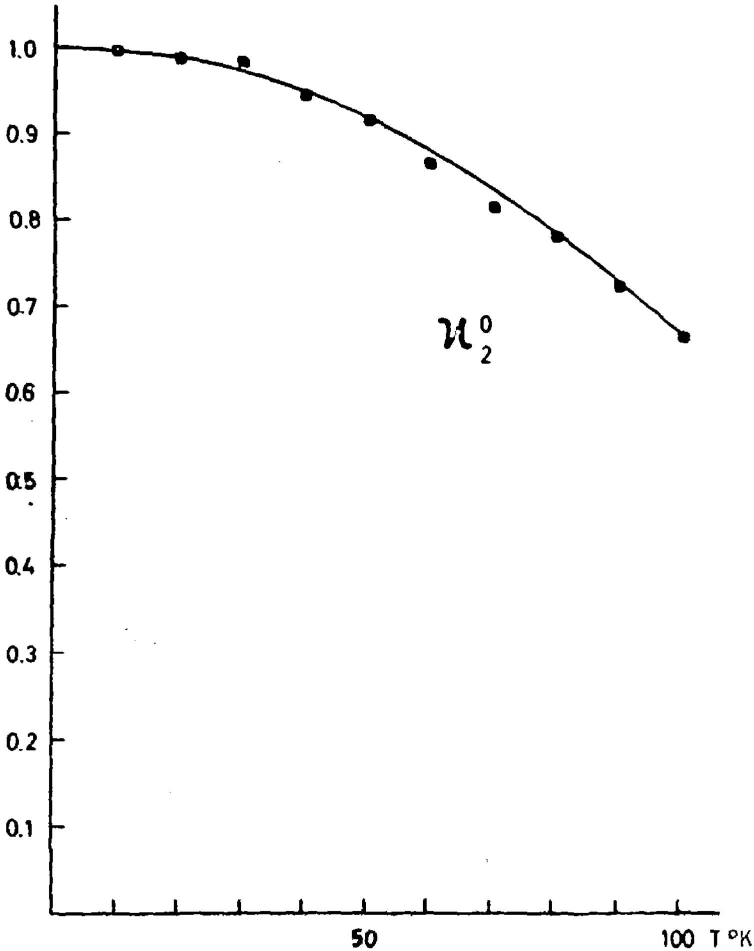

Fig 14. Anisotropy Coefficients, Tb comparison with experimental values

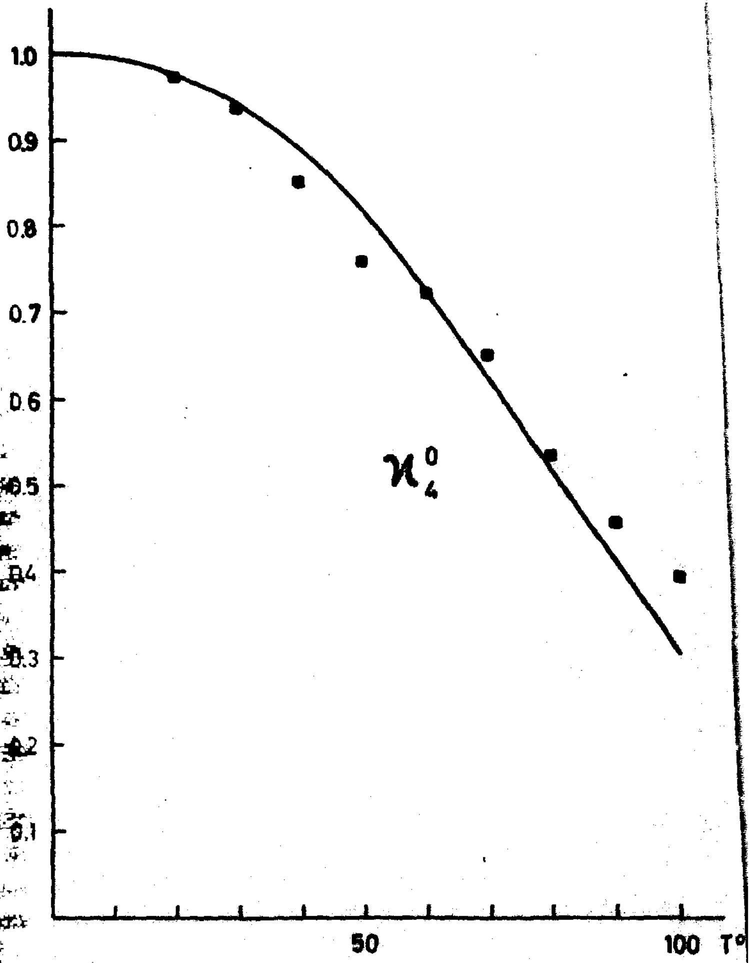

Fig 15. Anisotropy Coefficients, Tb. comparison with experimental values

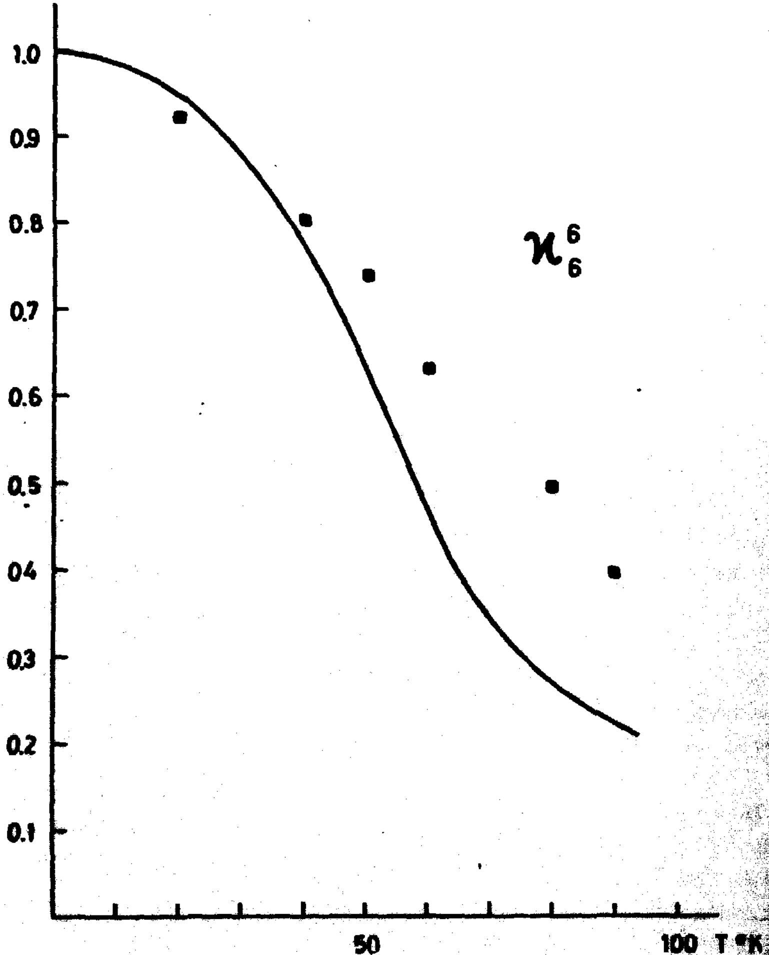

Fig 16. Anisotropy Coefficients, Tb. comparison with experimental values.