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TEMPERATURE DEPENDENCE OF MAGNETIC
ANISOTROPY AND MAGNETOSTRICTION:
BEYOND THE MEAN-FIELD THEORY



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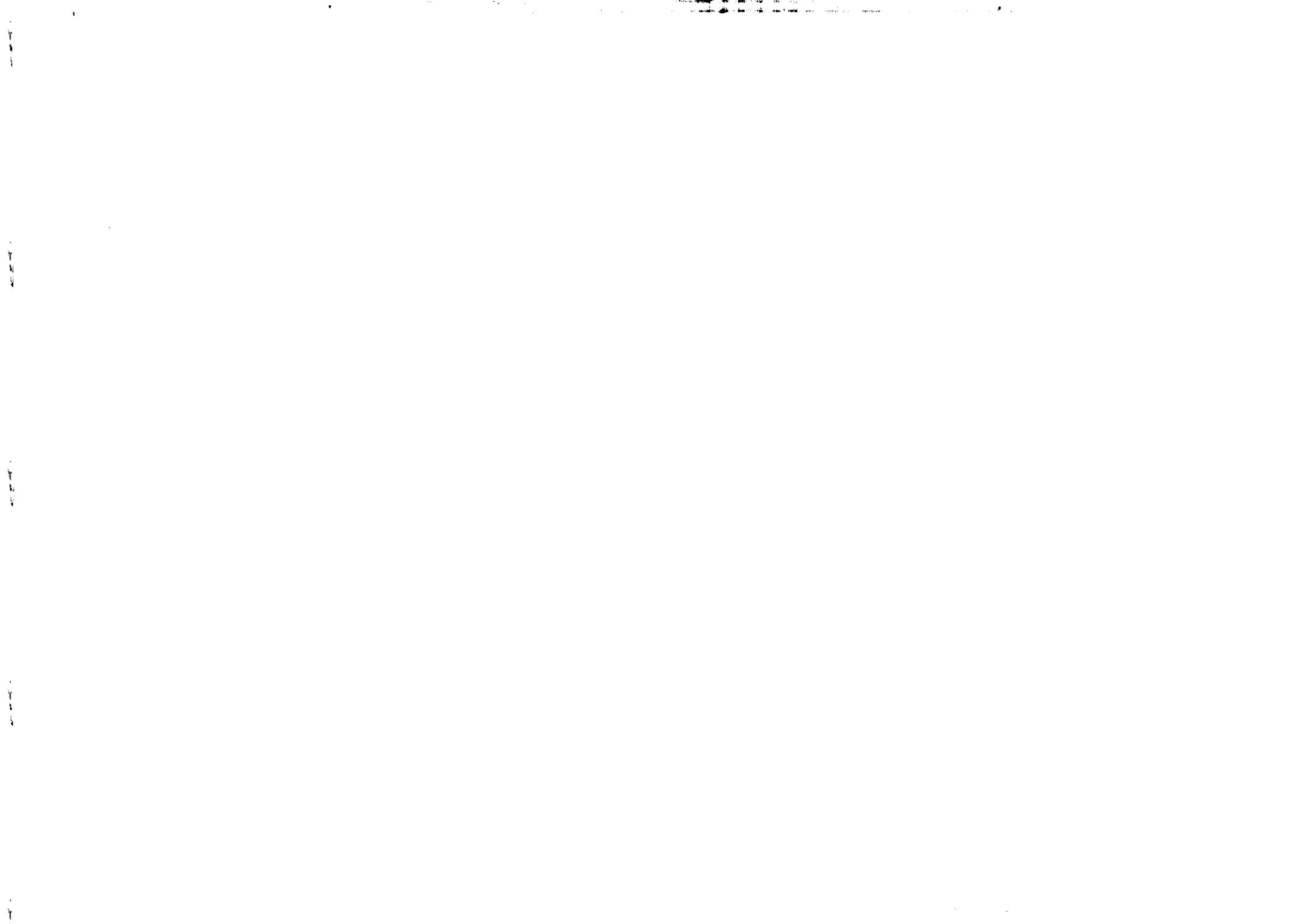
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MIRAMARE-TRIESTE



International Atomic Energy Agency
and
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**TEMPERATURE DEPENDENCE OF MAGNETIC ANISOTROPY
AND MAGNETOSTRICTION:
BEYOND THE MEAN-FIELD THEORY**

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Abstract.

The first nonvanishing *magnetic anisotropy coefficient* is calculated as a function of temperature for *any* spin quantum number and *all* temperatures below the Curie temperature for the case of face-centred cubic symmetry within the random-phase approximation (RPA). A detailed and instructive comparison between the mean-field and the RPA predictions is carried out. The RPA magnetization curves are also given for the first time for spins $S > 1/2$. Most of the theoretical considerations are quite general as regards lattice type and even decoupling scheme and can thus be applied straightforwardly to other cases of interest.

The progress reported here has been attained with the help of a new simplified and improved parametric approach and of a recent calculation of the average occupation number of magnons within the RPA. In particular, the new approach makes unnecessary the solving of integral equations so that the proposed procedure is especially simple and practically versatile in applications to any particular anisotropic material.

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1 Introduction

Very recently, the Callen and Callen theory of magnetic anisotropy and magnetostriction of single-ion origin (Callen and Callen 1965, du Tremolet 1993) was extended to the *quantum* case of finite spin number S of the localized magnetic moments (Millev and Fähnle 1994a). Besides, the theory was cast into the framework of the insightful theorem of Callen and Shtrikman (1965) and was thus potentially related not only to experiment via the eventual insertion at the final, phenomenological stage of the *experimental* temperature dependence of the magnetization in the system under consideration (Wolf 1957, Callen and Callen 1965), but also to the general class of theories defined by Callen and Shtrikman (1965). The expectation values (moments) of the type $M_n \equiv \langle S_j^n \rangle$ which are needed in the fundamental theory of Callen and Callen (1965) (du Tremolet 1993) can all be expressed within this framework as functions of the first moment M_1 or, equivalently, of the reduced magnetization $m = M_1/S$, the functional dependence $M_n = M_n(M_1)$ itself being model-independent for this class which encompasses the most important renormalized quasi-independent collective-excitation theories including the spin-wave (SW) theory, the random-phase approximation (RPA), some improved decoupling schemes in the Green's functions approach (Callen 1963, Tahir-Kheli 1975), and the mean-field (MF) theory.

It was shown (Millev and Fähnle 1994) that the *quantum* (finite- S) curves $M_n(M_1)$ are only seemingly close to each other and to the *classical* (infinite- S) curves (Callen and Callen 1965); this apparency has led until recently (Kuz'min 1992, Wolf et al 1994) to utilizing the classical curves $M_n(M_1)$ only. The proof of this observation was given by generating the MF temperature dependences of the first anisotropy coefficient κ_2 (Millev and Fähnle 1994): for any reasonable finite S , $\kappa_2(T)$ was demonstrated to be substantially different, both qualitatively and quantitatively, from the predicted *linear* classical temperature dependence.

It is the purpose of this paper to extend the study of the temperature dependence of anisotropy and magnetostriction by calculating explicitly $\kappa_4(T)$ within the RPA to the Green's functions approach to ferromagnetism for *any* S and for *all* $T \leq T_c$, thus providing for an untrivial theoretical prediction for the temperature dependence of the fundamentally and technologically important anisotropy characteristics. While most of the statements and results are quite general as regards the lattice type and even the decoupling scheme, in

order to remain within tolerable limits of space we discuss in full detail only the face-centred cubic (*fcc*) lattice case. In fact, the *fcc* case is more difficult than the simple-cubic (*sc*) and the body-centred (*bcc*) cases, so that we are tackling the trickiest case in cubic geometry. Besides, the extension to lower-symmetry lattices is quite straightforward. Furthermore, the calculation of the temperature dependence of the anisotropy coefficients is not the only important achievement reported below. It necessitates, and has forced us, to (i) calculate the required Bose-Einstein lattice sums for the average number of quasiparticle excitations (magnons) (Millev and Fähnle 1994b); (ii) simplify and extend the parametric approach of Millev and Fähnle (1994a,c); (iii) obtain, with the help of "(ii)", the magnetization curves $m(T)$ for *any* spin S within the RPA over the *entire* temperature range below the Curie temperature T_c . The significance of the last item should not be overlooked: to our knowledge, the only $m(T)$ -curves for all $T \leq T_c$ within any of the established Green's functions techniques are those for the *lowest* spin value of $S = 1/2$, although it is exactly this case where the predictions of these theories have been recognized as unsatisfactory, and pronouncedly so at very low temperatures (Tahir-Kheli and ter Haar 1962, Callen 1963). It seems that the reason for 'remaining low in spin' is the fact that the case $S = 1/2$ has the exceptional feature of providing a linear dependence between the average occupation number of magnons Φ and the magnetization m (Tahir-Kheli and ter Haar 1962, Callen 1963, Sauter 1963, Praveczi 1963) and this has been decisive for the numerical computation of $m(T)$ which involves the solution of an integral self-consistent expression (Tyablikov 1967). To put it plain, the simplified and extended parametric approach we introduce here renders unnecessary the solving of integral equations, thus making the proposed procedure especially simple, attractive, and versatile in *practical* applications for any particular anisotropic material.

2 The theoretical framework

The developments we suggest will now be introduced in the following natural way: One starts with the expressions for the magnetic anisotropy *coefficients* κ_2 and κ_4 as functions of the moments M_2 and M_4 (Callen and Callen 1965,

du Tremolet de Lacheisserie 1993) and goes ahead step by step until, finally, the dependence on the temperature is calculated. Before doing this, note that (i) the widely used anisotropy constants K_1 and K_2 are simple linear combinations of the coefficients κ_i (Birss 1966, du Tremolet 1993); (ii) in materials of cubic symmetry, κ_2 and K_1 are identically zero; (iii) the magnetostriction coefficients are calculated within the prescriptions of the well-established theory of the Callens (1965) and are given by linear combinations involving the averages of the moments M_n .

2.1 The anisotropy coefficients as functions of the moments M_n

The anisotropy coefficients κ_l are defined as the normalized averages of the tensor operators T_l^n (Callen and Callen 1965, Bowden et al 1986):

$$\kappa_2 = \frac{\langle T_2^0 \rangle}{\langle T_2^0 \rangle_{|T=0}}, \quad \kappa_4 = \frac{\langle T_4^0 \rangle}{\langle T_4^0 \rangle_{|T=0}}. \quad (1)$$

Starting with a general Hamiltonian

$$\hat{H} = \hat{H}_{ex} + \hat{H}_Z + \hat{H}_{cf} \quad (2)$$

with the first two terms representing the isotropic exchange between the spins and the usual Zeeman term, respectively, and the last term being the single-ion anisotropy term, one assumes that $\hat{H}_{cf} \ll \hat{H}_{ex} + \hat{H}_Z$ and treats the anisotropy as a small perturbation on the dominant exchange interaction. To first order of the thermodynamic perturbation theory, one obtains for the free energy

$$F = F_0 + \langle \hat{H}_{cf} \rangle. \quad (3)$$

With the assumption for the single-ion character of the anisotropy and on using well-known relations between the components of the vector spin operators (Callen and Shtrikman 1965), the problem is reduced to the calculation of the expectation values $\langle (\hat{S}_j^z)^n \rangle$ of the z -component only. To avoid unnecessary complications, we discuss only crystalline materials, or a particular sublattice, with spins sitting on equivalent sites and, hence, we drop the site index j .

The first two anisotropy coefficients which are, with the exception of hexagonal symmetry, the only relevant ones are given by (Bowden et al 1986)

$$\begin{aligned} \kappa_2 &= \frac{\langle T_2^0 \rangle}{\langle T_2^0 \rangle_{|T=0}} = \frac{3M_2 - S(S+1)}{S(2S-1)} \quad (S \geq 1), \quad (4) \\ \kappa_4 &= \frac{\langle T_4^0 \rangle}{\langle T_4^0 \rangle_{|T=0}} = \frac{35M_4 - 5(6S^2 + 6S - 5)M_2 + 3(S+2)(S+1)S(S-1)}{8S(S-\frac{1}{2})(S-1)(S-\frac{3}{2})} \quad (S \geq 2), \quad (5) \end{aligned}$$

where the restrictions for the values of S reflect the underlying quantum-mechanical property of the combinations of powers of spin operators in the definitions of the κ 's. The restrictions do not imply that materials with sufficiently low values of S cannot exhibit magnetic anisotropy: it is the single-ion contribution that vanishes, while pair-interaction contributions might still be present.

2.2 Computation of the moments M_n as functions of the generalized effective field x

One of the crucial points in the anisotropy theory of Callen and Callen (1965) is the elucidation of the fact that the higher moments M_n can all be expressed as functions of the reduced magnetization $m = M_1/S$, whereby the temperature T and the magnetic field H enter indirectly via $m = m(T, H)$. The latter dependence could then be taken from experiment and inserted into the theoretically calculated M_n 's with $n > 1$. In many cases this procedure avoids disastrous discrepancies with experiment which occur when one persists to carry out the calculation self-consistently in the mean-field approximation and to insert the mean-field result for $m = m(T, H)$ which is known to be unsatisfactory except in some particular cases. A remarkable generalizing insight was provided by Callen and Shtrikman (1965), who revealed that the source of the success of the semi-phenomenological approach stems from the fact that the functional dependence $M_n = M_n(M_1)$ is model-independent in all renormalized quasi-independent collective-excitation theories including the spin-wave theory, the random-phase approximation, the improved interpolation decoupling schemes in the Green's functions approach, and the

mean-field theory itself. It was shown that for all these theories the relevant information can be presented most compactly by considering the moments' generating function

$$\Omega_S(a, x) \equiv \langle \exp(a\hat{S}_z) \rangle_0 = \frac{\sinh[\frac{1}{2}(2S+1)(a+x)]}{\sinh[\frac{1}{2}(a+x)]} / \frac{\sinh[\frac{1}{2}(2S+1)x]}{\sinh \frac{x}{2}} \quad (6)$$

and the equation for the first moment $M_1 \equiv \langle \hat{S}^z \rangle_0 = mS$:

$$M_1(x) = SB_S(xS), \quad (7)$$

where

$$B_S(y) = \alpha \coth(\alpha \cdot y) - \beta \coth(\beta \cdot y) \quad (\alpha = \frac{2S+1}{2S}, \beta = \frac{1}{2S}) \quad (8)$$

is the Brillouin function, while x is the generalized effective field given by

$$x = \ln(1 + \frac{1}{\Phi}) \quad (9)$$

with the average occupation number of quasiparticles Φ defined as usual by

$$\Phi = \frac{1}{N} \sum_{\mathbf{p}} \frac{1}{\exp(\epsilon_{\mathbf{p}}/k_B T) - 1}; \quad (10)$$

$\epsilon_{\mathbf{p}}$ is the energy spectrum of the excitations as a function of the momenta \mathbf{p} .

Bringing the self-consistent equation for M_1 into the form (7) was an untrivial step based on the ingenious substitution

$$\Phi = \frac{1}{\exp(x) - 1} \quad (11)$$

(cf Eq.(9)) and on knowledge of the algebraic connection between M_1 and Φ for all values of S (Callen 1963, Sauter 1963, Praveczi 1963). Now then any moment is calculated from the generating function by simple differentiation:

$$M_n(x) = \frac{\partial^n}{\partial a^n} \Omega_S(a, x)|_{a=0}. \quad (12)$$

The Callen and Shtrikman programme is formally accomplished by examining together $M_1(x)$ and $M_n(x)$, whereby

$$x = \frac{1}{S} B_S^{-1}(m) \quad (13)$$

and, consequently,

$$M_n = M_n(\frac{1}{S} B_S^{-1}(m)). \quad (14)$$

Recently, it was shown (Millev and Föhnle 1992a,b) that the inverse Brillouin function B_S^{-1} is a logarithmic one,

$$B_S^{-1}(m) = S \ln z^*(m), \quad (15)$$

where z^* is the unique positive root of the polynomial equation

$$\sum_{k=0}^{2S} [(m+1)S - k] z^k = 0 \quad (16)$$

By comparison of Eqs.(9) and (15),

$$x = z(m) = \ln(z^*(m)), \quad (17)$$

i.e.,

$$z^*(m) = 1 + 1/\Phi. \quad (18)$$

The last relation gives the unique root z^* a clear physical meaning in terms of the average number of magnons. Thus, the generating function can be given directly in terms of $z^*(m)$ or of Φ . In particular, $\Omega_S(a, z^*(m))$ is reduced to an algebraic function in z^* :

$$\Omega_S(a, z^*(m)) = e^{-aS} \frac{G(z^*, a)}{G(z^*, 0)}, \quad (19)$$

where $G(z^*, a)$ is the geometric progression

$$G(z^*, a) = \sum_{k=0}^{2S} (z^* e^a)^k. \quad (20)$$

One easily finds that

$$M_n(z^*(m)) = \frac{1}{G(z^*, 0)} \sum_{l=0}^n \frac{n!}{(n-l)!} (-S)^{n-l} \frac{\partial^l G(z^*, a)}{\partial a^l} \Big|_{a=0}. \quad (21)$$

The root $z^*(m)$ up to $S = 3/2$ is given in Millev and Föhnle (1992a, 1994a) and so the analytic solution of the anisotropy problem is explicit up

to this value of spin. However, as mentioned above, in *cubic* systems $\kappa_2 \equiv 0$ and, besides, anisotropy can only be supported for sufficiently high values of spin $S \geq 2$. In other words, the *first* anisotropy coefficient in materials of cubic symmetry is κ_4 from Eq.(5) with $S \geq 2$. In fact, the problem was solved for any value of spin by invoking a parametric solution for the self-consistent equation for the magnetization (Millev and Fähnle 1994a,b).

3 An improved parametric method to solve the anisotropy problem

3.1 The anisotropy coefficients as functions of the magnetization

The parametric approach suggested by Millev and Fähnle (1994c) is as explicit and analytic as possible, i.e. it gives explicit expressions at the intermediate stages of the calculation. This notwithstanding, at the end one still has to use a purely numerical procedure. So, from the point of view of getting the final result in a tabular or graphical form, the intermediate stage is redundant. This point has already been commented upon (Millev and Fähnle 1994a,d). The most straightforward and effective way is to use as a parameter *the generalized effective field x itself*. It is so much the better that this parameter has a clear physical meaning, thus resembling the entropy difference parametrization of Lekner (1982) in a parametrical solution relevant to the critical point of a liquid. In fact, the only knowledge about the generalized effective field x which is required to carry out the computations is that x sweeps between 0 and infinity, the left limit being attained for very (infinitely) high temperatures in zero external field, while the right limit corresponds to zero temperature and arbitrary (including zero) external field. Besides, the variation of x with temperature is monotonic, provided the external field is held fixed numerically *and* experimentally. It can, of course, be absent. Summarizing all these considerations, the simplified parametric method we now suggest amounts to the following formal procedure: Let x

sweep between 0 and ∞ , compute $M_1(x)$ (i.e. $m(x)$) from Eq.(7), compute κ_2 and κ_4 from Eqs.(4)-(5) by using $M_2(x)$ and $M_4(x)$ from Eq.(21). Finally, collect pairs of computed points, corresponding to the same value of x , to plot or tabulate κ_2 and κ_4 .

3.2 The temperature dependence of the anisotropy coefficients

In principle, the outlined parametric approach will produce just as easily the temperature dependence of the required quantities whenever the "temperature part" in the generalized effective field x can be separated (factorized out) from the rest, i.e. from the magnetization and external field dependence (Millev and Fähnle 1993). Not unexpectedly, within the class of theories considered here this separation is straightforward for, and the parametric procedure is immediately applicable to, the MF theory of ferromagnetism only. There,

$$x = \frac{3}{S+1} \cdot \frac{m}{t}, \quad (22)$$

where $t \equiv T/T_c$ and T_c is the MF Curie temperature. Hence,

$$t = t(x) = \frac{3}{S+1} \cdot \frac{m(x)}{x} \quad (23)$$

and the computation proceeds as before with x sweeping between $[0, \infty)$. Now one may collect pairs of points corresponding to the same value of x to get $m(T)$, $M_2(t)$, $M_4(t)$, $\kappa_2(t)$, $\kappa_4(t)$ or whatever other dependence *parametrized by x* which might be interesting, e.g., $\kappa_2(m)$, etc. This straightforward procedure was tested and found computationally superior both close to $T = 0$ and to $T = T_c$ when compared with the parametrization used by Millev and Fähnle (1994a,c). This observation reflects back to those problems whose treatment was suggested in the last two papers.

The intriguing point in the problem with the temperature dependence of anisotropy and magnetostriction is how to get the temperature dependence in a *nontrivial* theory from among the discussed class of quasiparticle-excitations theories. We now turn to this problem within the more elaborate scheme of the Green's functions approach (Tyablikov 1967, Tahir-Kheli

1975). The scheme of reasoning will be to express *all* relevant quantities as explicit functions of a parameter Q which plays the same part in the calculation of the *temperature* dependence of the anisotropy coefficients as that played by the generalized effective field x in the calculation of the dependence of anisotropy on *magnetization* (see previous subsection).

4 Calculation of the average occupation number Φ of quasiparticle excitations within the RPA

A new method for the calculation of Φ valid for *any* type of lattice was proposed very recently (Millev and Föhnle 1994b). The method is based on the recognition of the connection of the problem with lattice Green's functions and generalized Watson integrals, on one hand, and on a very simple differentiation technique. The results have been specified completely for the three cubic cases. While a comparison between the different cubic cases might be rewarding as regards the tracing down of subtle geometric effects, we postpone this issue for further investigation and concentrate on the *fcc* case. It is the most difficult of the three and thus provides for a kind of an upper bound for the amount of labour involved in cubic symmetry at least.

Starting with the definition (10), one introduces the above-mentioned parameter Q as:

$$Q: \quad \epsilon(\mathbf{k})/k_B T \equiv 2Q(1 - \gamma_{\mathbf{k}}) \quad (0 \leq Q \leq \infty), \quad (24)$$

where the dispersion is determined by

$$\gamma_{\mathbf{k}} = J(\mathbf{k})/J(0), \quad (25)$$

and

$$J(\mathbf{k}) = \sum_{\mathbf{R}_{n,n}} J(\mathbf{R}) \exp i\mathbf{k} \cdot \mathbf{R} \quad (26)$$

is the Fourier transform of the *nearest-neighbour* ferromagnetic exchange coupling between moments sitting on sites \mathbf{f} and \mathbf{g} ($R_{n,n} = \mathbf{f} - \mathbf{g}$). The sum to be calculated is now cast as

$$\Phi(Q) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\exp[2Q(1 - \gamma_{\mathbf{k}})] - 1} \quad (27)$$

and the summation is over all reciprocal-lattice vectors \mathbf{k} in the first Brillouin zone of the crystal with N sites. As the calculation has already been presented in sufficient detail (Millev and Föhnle 1994b), here we give only the relevant final results. One finds that

$$\Phi(Q)_{fcc} = \Phi_0 + \frac{1}{2} \sum_{k=1}^{\infty} (-1)^k A_k \frac{Q^k}{k!} \frac{d^k}{dQ^k} (\coth Q), \quad (28)$$

where

$$\Phi_0 = \frac{1}{\exp(2Q) - 1} \quad (29)$$

and the coefficients A_k are defined via the triple trigonometric integrals

$$A_k(fcc) = \frac{1}{\pi^3} \frac{1}{3^k} \int \int \int_0^\pi dx_1 dx_2 dx_3 (\cos x_1 \cos x_2 + \cos x_2 \cos x_3 + \cos x_3 \cos x_1)^k. \quad (30)$$

A special procedure was developed for the calculation of the A_k 's (Millev and Föhnle 1994b). They can be found from

$$A_k = \sum_{q=0}^k c_{k-q} c_q \quad (31)$$

with the c_n 's calculated from the three-position recursion relation (Joyce 1973)

$$c_{n+1} = \frac{n}{6(n+1)^2} [(4n+1)c_n + (2n-1)c_{n-1}]. \quad (32)$$

The required sum $\Phi(Q)$ is thus completely specified by the convergent expansion (28) supplemented with Eqs.(31-32) for the A_k 's. Remarkably, $\Phi_0(Q)$ corresponds precisely to the MF approximation and this is so much the more evident if one considers the insightful analogy between the MF theory of ferromagnetism and the Einstein (degenerate-spectrum) phonon theory (Callen and Shtrikman 1965). Furthermore, the same argument allows to interpret

physically the parameter Q ($0 \leq Q \leq \infty$). Namely, on comparing the expression

$$\Phi = \frac{1}{\exp(x) - 1} \quad (33)$$

which follows from Eq.(9) with Φ_0 from Eq.(29), one immediately identifies $Q = x/2$. Therefore, Q is simply proportional to the generalized effective field x in the MF approximation which emerges as the zeroth term in the systematic expansion (28) of the average occupation number of magnons. This proportionality does not hold beyond the MF level (see Fig.1).

Note however that the discussion up to this stage is completely general and valid for the *whole* class of theories defined by Callen and Shtrikman (1965). The reason is that we introduced, intentionally, the flowing parameter Q quite formally by Eq.(24). It is also obvious that Q will depend on the particular renormalization of the quasiparticle excitation spectrum and it is, of course, sensitive to the adopted decoupling scheme. We proceed with the RPA theory, postponing for a further investigation the treatment within some more involved decoupling schemes.

Comparing our formal definition of Q (Eq.(24)) with the renormalized energy spectrum in the RPA approximation (Tahir-Kheli and ter Haar 1962, Tahir-Kheli 1975), we find

$$Q = \frac{3P(1)}{2S(S+1)} \cdot \frac{\langle S^z \rangle}{t} = \frac{3P(1)}{2(S+1)} \cdot \frac{m}{t}, \quad (34)$$

where m and t are, as above, the reduced magnetization and temperature and $P(1) = 1.34466$ is the Watson integral for the *fcc* lattice (Watson 1939). The appearance of the peculiar numerical factor of $P(1)$ is due to the fact that in the RPA the critical temperature coincides with that for the spherical model of ferromagnetism (Tahir-Kheli and ter Haar 1962, Joyce 1972) and is $P(1)$ times lower than the respective MF critical temperature. Solving Eq.(34) for t , one gets

$$t = t(Q) = \frac{3P(1)}{2(S+1)} \cdot \frac{m(Q)}{Q}. \quad (35)$$

The last equation completes the scheme for the implementation of the parametric method of subsection 3.2, the computations now being run with the flowing parameter Q .

To summarize the salient features of the procedure, we forget for a while *how* the things were effected and emphasize *what* are the relevant results. Thus, sticking to the general notion of the functional connection, what we calculated explicitly was:

$$\Phi = \Phi(Q), \quad (36)$$

$$M_n = M_n(x(\Phi(Q))) = M_n(Q), \quad (37)$$

$$\kappa_l = \kappa_l(M_m(x(\Phi(Q)))) = \kappa_l(Q), \quad (38)$$

$$t = t(m(Q), Q) = t(Q). \quad (39)$$

The temperature dependences $\Phi(t)$, $m(t)$, $M_n(t)$, $\kappa_l(t)$ within the RPA and without an external magnetic field are now simply generated in a graphical or tabular form by collecting pairs of points corresponding to the same value of the parametrizing quantity Q . Note, once again, that the specific decoupling scheme enters the last relation only. Besides, now that everything which is physically meaningful in the problem has been parametrized, one can generate any other mutual dependence as, e.g., $\Phi(m)$ or vice versa, etc.

5 Results and discussion

It should have become evident from the above that not only is the problem with the temperature dependence of the anisotropy coefficients within the RPA and in a *fcc* lattice solved, but also other important and unreported information can be deduced without much effort. Here we report only the most significant results leaving aside for the time being other possible applications of the method. It should also be clear that one must specify the order in k in Eq.(28), up to which the summation for $\Phi(Q)$ has been carried out. Below, we report results up to and including $k = 6$. There is no problem to carry out the numerical computations to *any* k , because all quantities are easily

calculable following work by Millev and Fähnle (1994b) (the only problem which remained unexplained so far is whether there exists an expression for the derivatives of $\coth(x)$ which would allow a straightforward algorithmization; such an expression is provided, for instance, by Wintucky (1973)). The sum for $\Phi(Q)$ is convergent fast enough except at very low temperatures (large Q). Working up to $k = 6$ gives for very low temperatures ($Q \approx 5$) average number of magnons of the order of 10^{-3} which is of the order of magnitude found in the asymptotically exact SW theory (Dyson 1956) (to leading order in $t = T/T_c$, both the RPA and Dyson's theory give the famous Bloch $T^{3/2}$ -law (Kronmüller and Lambeck 1992)). We thus conclude that for any practical purposes the order in k we considered provides for sufficient accuracy at all temperatures below T_c .

Firstly, in Fig.2 we give the temperature dependence, in reduced units, of the magnetization $m(T)$ in the RPA for all S between $1/2$ and $7/2$. Any other S can be just as easily calculated. We believe that already these results are not known for $S > 1/2$. One is, of course, interested to compare the RPA with the MF prediction for $m(T)$. More than this can be seen in Fig.3, where $m(T)$ is given as calculated to different order in k ; only the even k 's up to 6 for the representative value of $S = 1$ have been displayed to make the plots discernible. The extreme plots ($k = 6$ and $k = 0$, resp.) correspond to the RPA to this high order in k and to the MF result. While it can be argued that the difference is not very large in reduced units, the RPA magnetization is systematically smaller. Since the magnetization curves for *different* values of spin in both the MF and RPA are monotonically arranged (the smaller the spin, the higher the curve), it might be remarked that working in the cruder (MF) approximation for a *given* spin is effectively equivalent to working in the finer (RPA) theory with *some smaller* spin, if such is allowed.

The central group of results, however, concerns the temperature dependence of the anisotropy coefficient κ_4 which is the *first* nonvanishing coefficient in cubic (here: *fcc*) symmetry. We give first the MF anisotropy curves for $S = 2, 5/2, 3, 7/2$ (Fig.4) which are new results in themselves. Next, we give the temperature dependence of anisotropy in the RPA for the same values of spin (Fig.5). To compare more clearly the predictions of both approximations, in Fig.6 we present the anisotropy coefficient κ_4 for a given value of S , $S = 5/2$. Some features of this comparison are common for all values of spin. Firstly, the MF result overestimates the anisotropy, and especially so at low temperatures. There, the RPA result is practically exact and

reflects the correct account for the spin waves at low temperatures. Secondly, both theories give asymptotically identical results, which is not unexpected since the underlying asymptotic temperature dependences of the magnetization as $T \rightarrow T_c$ are identical with the MF critical exponent $\beta = 1/2$. Finally, the higher the spin, the smaller the difference between both approximations. It is certainly interesting that within the very general theory we exploit the temperature dependence of anisotropy in *fcc* materials has the peculiar bell shape, the bells being pronouncedly "slimmer" in the RPA as explained above. More precisely, in contrast to the first anisotropy coefficient κ_2 in non-cubic crystalline materials, in cubic materials the respective curves have an inflexion point approximately half way down from the Curie temperature. This holds for both the MF and the RPA theories. Qualitatively similar dependences for the anisotropy *constants* have recently been measured in novel hard magnetic materials like $RE_2Fe_{17}N_x$ and $Sm_2Fe_{17}C_{3-\delta}$, though in symmetry lower than cubic (du Tremolet 1994, Xu et al 1993, Li and Cadogan 1992). The underlying reason for this similarity might be quite general and, possibly, independent of the type (soft or hard) of the magnetic material. One self-suggesting way of investigating into the problem is to use the present method together with the extension of the Callen and Shtrikman approach to the case of strong anisotropy (Bowden and Martin 1990).

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Figure Captions:

Figure 1:

Connection between the generalized effective field x and the flowing parameter Q . The dependence is linear only in the MF regime near the origin (small Q , $T \rightarrow T_c$), where $x = 2Q$ (see text).

Figure 2:

Temperature dependence of the magnetization $m(T)$ in the RPA. The curves 1 through 7 correspond to spins one half through seven halves. The curves for $S > 1/2$ are reported for the first time. Note that our method does not evoke numerical solution of integral expressions.

Figure 3:

The effect of orders in k on the temperature dependence of magnetization: curves 1 through 4 correspond to $k = 6, 4, 2$, and 0 , resp. The highest curve is the MF prediction.

Figure 4:

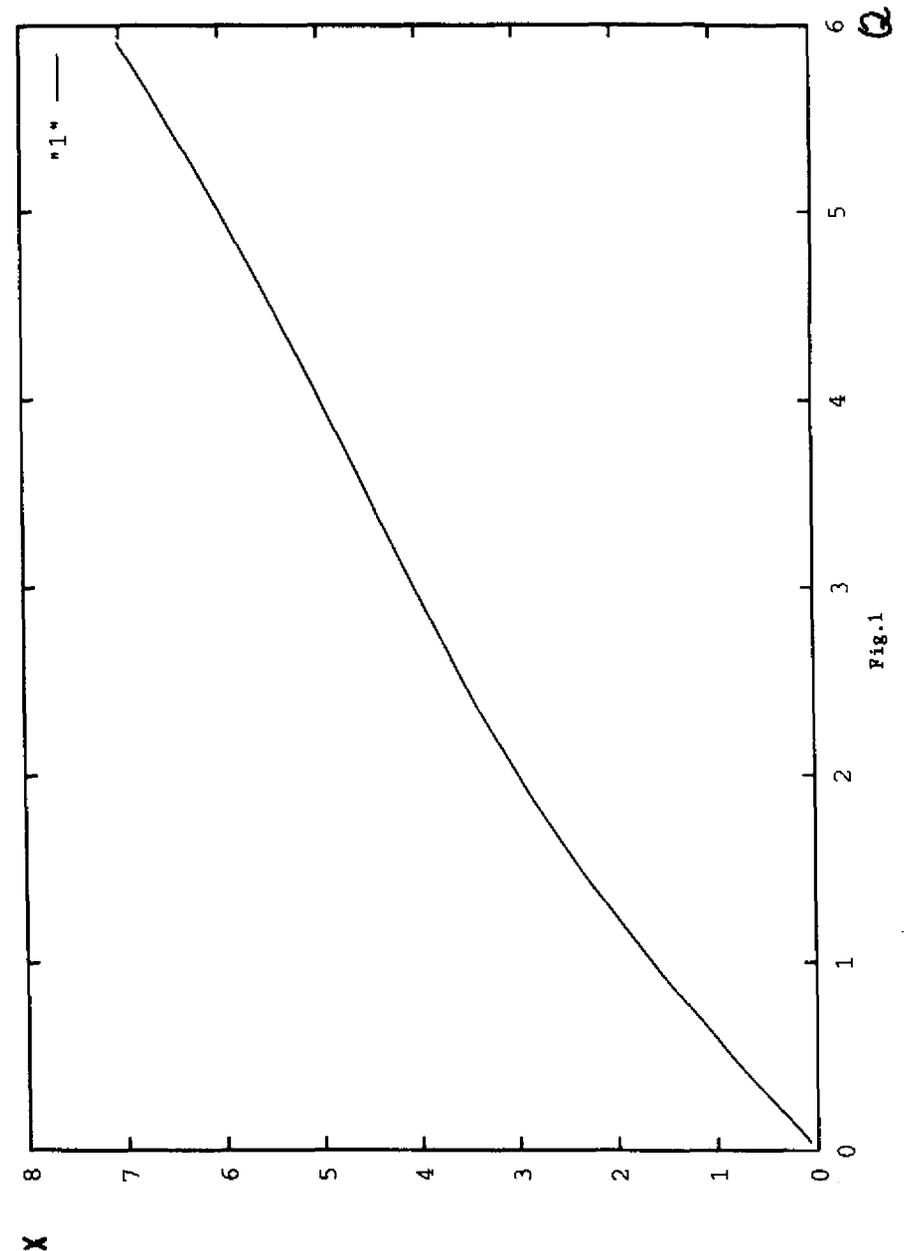
MF temperature dependence of the first non-vanishing anisotropy coefficient $\kappa_4(T)$: curves 1 through 4 correspond to $S = 2, 5/2, 3$, and $7/2$, resp.

Figure 5:

RPA prediction for $\kappa_4(T)$. The curves are arranged as in Fig.4. Note the bell shape and the fact that anisotropy curves even for neighbouring spin values lie quite distinctly apart despite the proximity of the corresponding magnetization curves $m(T)$ (see Fig.2).

Figure 6:

Comparison of $\kappa_4(T)$ within MF and RPA: $S = \frac{5}{2}$. MF overestimates the anisotropy, and especially so at low temperatures. Both approximations converge for $T \rightarrow T_c$.



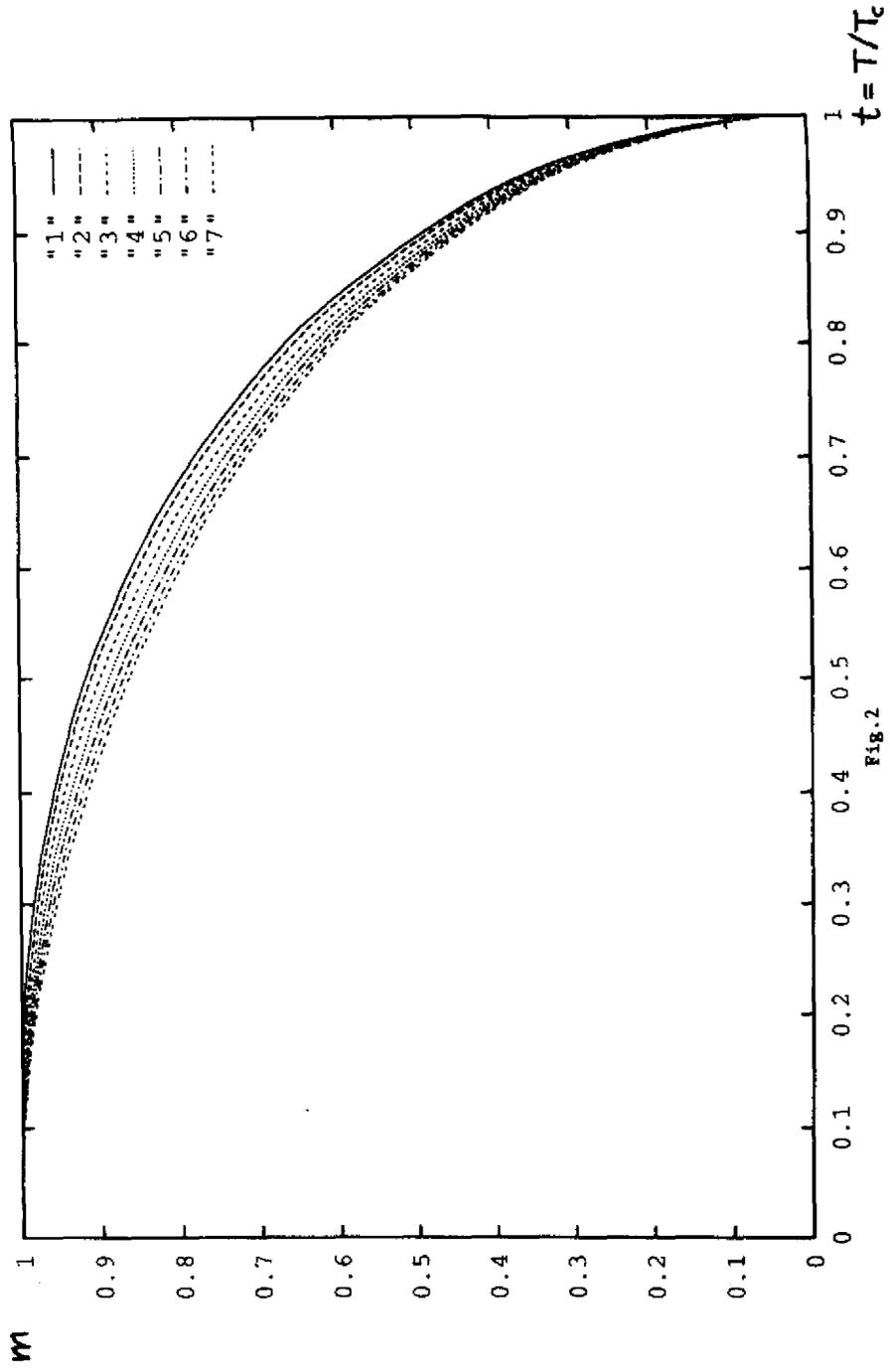


FIG. 2

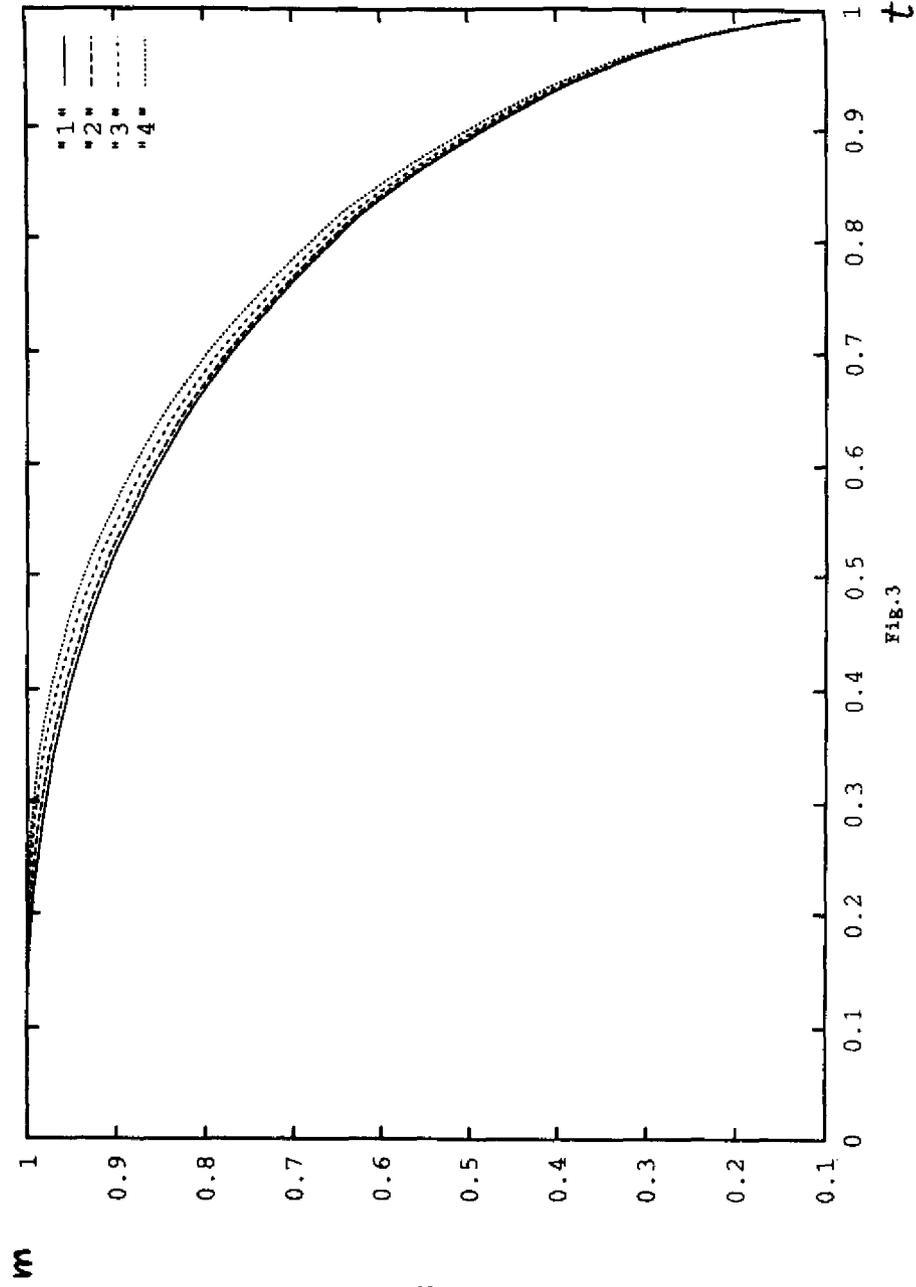
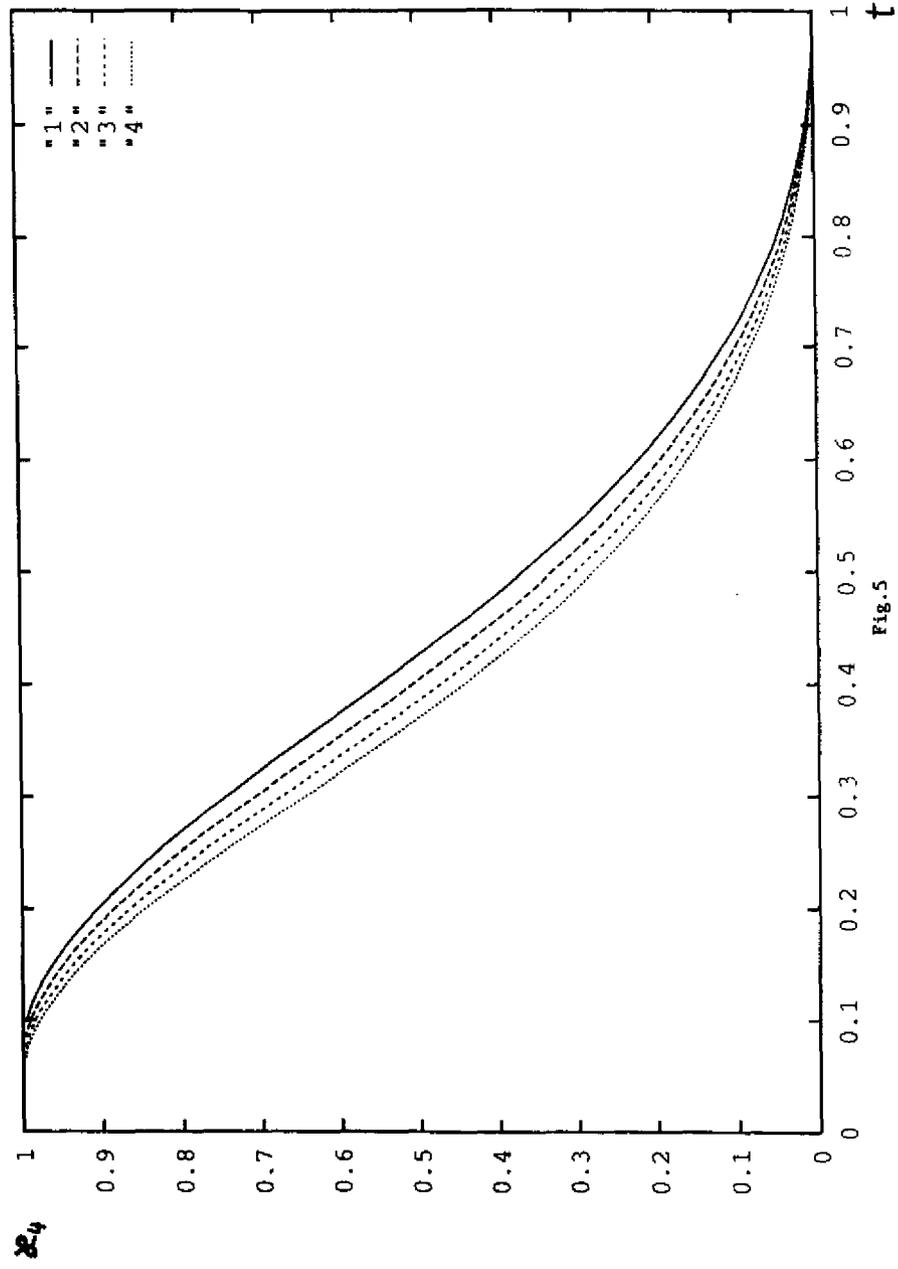
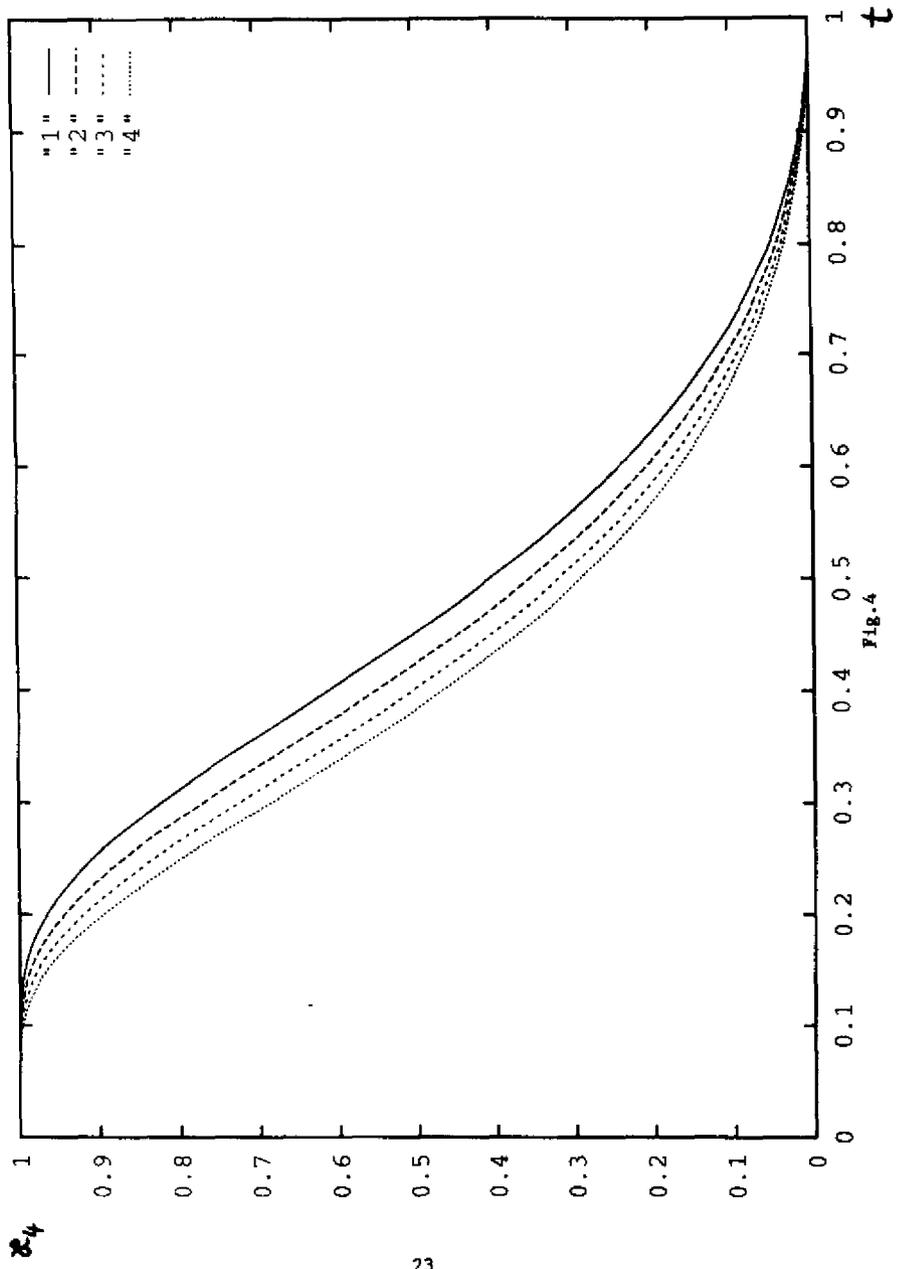


FIG. 3



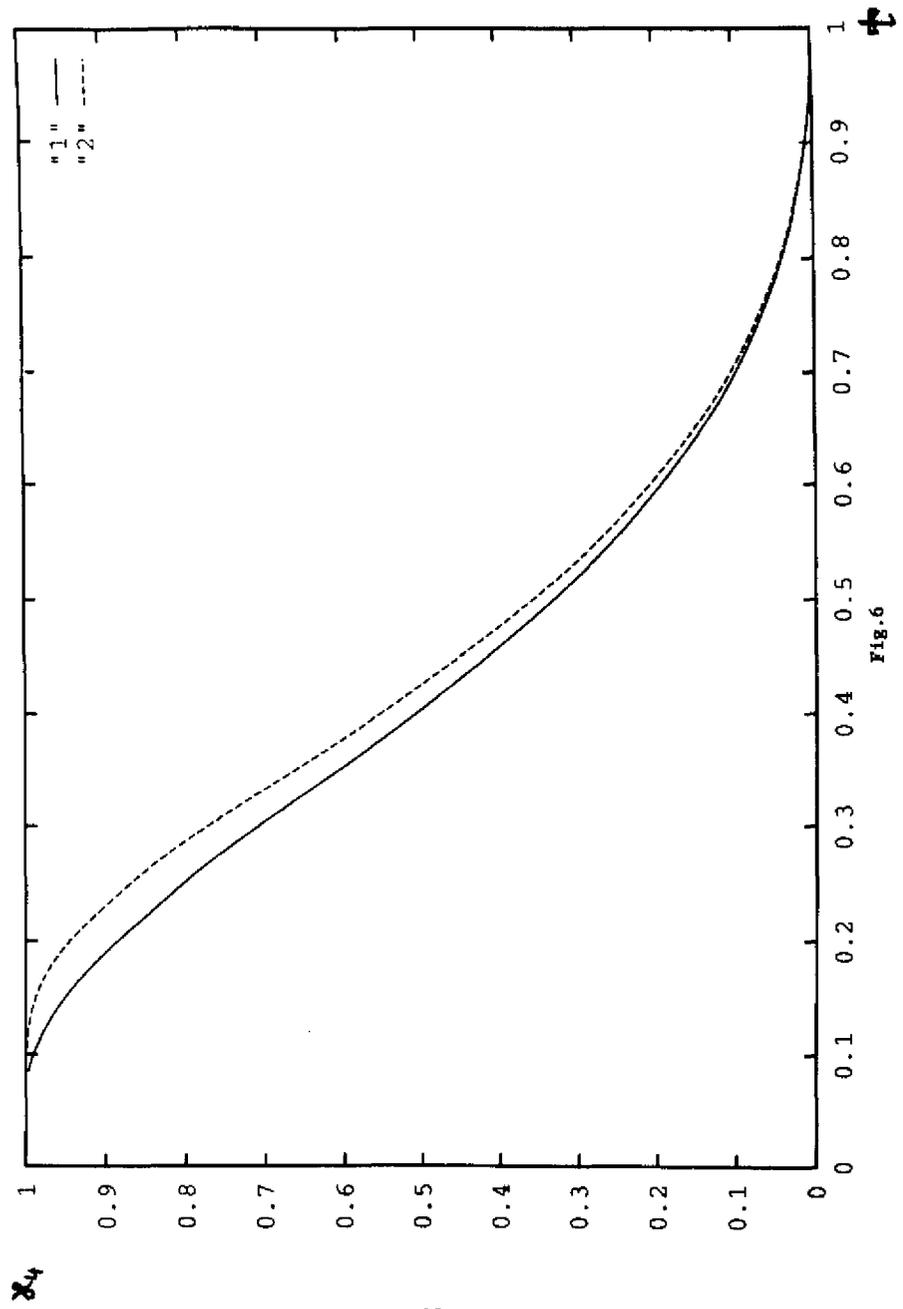


Fig. 6

