Temperature dependence of magnetic anisotropy and magnetostriction

Yonko Millev*
International Centre for Theoretical Physics, Condensed Matter Group, 34100 Trieste, Italy

Manfred Fähnle
Institut für Physik, Max-Planck-Institut für Metallforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Federal Republic of Germany
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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-centered 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 spins $S > \frac{1}{2}$. 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 simplified and improved parametric approach and of a recent calculation of the average occupation number of quasiparticle excitations within the RPA. In particular, this 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.

I. INTRODUCTION

Very recently, the Callen and Callen theory of magnetic anisotropy and magnetostriction of single-ion origin[1,2] was extended to the *quantum* case of finite spin number S of the localized magnetic moments.[3] Besides, the theory was cast into the framework of the insightful theorem of Callen and Shtrikman[4] 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,[5,1] but also to the general class of theories defined by Callen and Shtrikman.[4] The expectation values (moments) of the type $M_n \equiv \langle (\hat{S}_j^z)^n \rangle$, which are needed in the fundamental theory of Callen and Callen, 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 theory, the random-phase approximation (RPA), some improved decoupling schemes in the Green's-function approach,[6,7] and the mean-field (MF) theory.

It was shown[3] that the *quantum* (finite-S) curves $M_n(M_1)$ are only seemingly close to each other and to the *classical* (infinite-S) curves;[1] this apparency has led until recently[8,9] 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:[3] 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-function 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-centered-cubic (fcc) lattice case. In fact, the fcc case is more difficult than the simple-cubic (sc) and the body-centered (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);[10] (ii) simplify and extend the parametric approach of Refs. 3 and 11; (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 $S = \frac{1}{2}$, although it is exactly this case where the predictions of these theories have been recognized as unsatisfactory at very low temperatures.[12,6] It seems that the reason for "remaining low in spin" is the fact that the case $S = \frac{1}{2}$ has the exceptional feature of providing a simple dependence between the average occupation number of quasiparticles Φ and the magnetization m,[12,6,13,14] and this has been decisive for the numerical computation of

$m(T)$ which involves the solution of an integral self-consistent expression.[15] 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.

II. THE THEORETICAL FRAMEWORK: ITS "UNIVERSAL" PART

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 and goes ahead step by step until, finally, the dependence on the temperature is calculated.

The discussion of the theoretical framework is quite naturally divided into a "universal" part (which is described in this section) and a "particular" part (to which the next section is devoted). The universal part goes as far as the determination of the anisotropy coefficients as functions of magnetization: these functions are identical for the whole class of theories which share the common probability density described in Ref. 4. Correspondingly, the curves $\kappa_2(m)$ and $\kappa_4(m)$ are common to the whole class and have already been given for finite S in Ref. 3. The particular part, described in the next section, refers to the *temperature* dependence of the first nonvanishing anisotropy coefficient κ_4 in cubic materials (only the fcc case will be discussed below).

In this part of the theoretical description, the individuality of the member theories of the class shows up via the specific dependence of magnetization on temperature and it is this dependence which has to be inserted into the universal results to bring the whole calculation to the desired end.

Before plunging into the discussion, the following general remarks have to be made: (i) the widely used anisotropy *constants* K_1 and K_2 are simple linear combinations of the *coefficients* κ_l;[16,2] (ii) in materials of *cubic* symmetry, κ_2 does not contribute; (iii) the *magnetostriction* coefficients are calculated within the prescriptions of the well-established theory of the Callens[1] and are given by linear combinations involving the averages of the moments M_n.

A. 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_q^n:[1,17]

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

Starting with a general Hamiltonian

$$\hat{H}=\hat{H}_{\rm ex}+\hat{H}_Z+\hat{H}_{\rm cf} \tag{2}$$

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 $\hat{H}_{\rm cf}\ll\hat{H}_{\rm ex}$ 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

$$F=F_0+\langle\hat{H}_{\rm cf}\rangle\ . \tag{3}$$

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,[1] 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[17]

$$\kappa_2=\frac{\langle T_2^0\rangle}{\langle T_2^0\rangle_{|T=0}}=\frac{3M_2-S(S+1)}{S(2S-1)}\quad (S\geq 1)\ , \tag{4}$$

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

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.

B. 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[1] 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[4] who revealed that the source of the success of the semiphenomenological 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 RPA, the improved interpolation decoupling

schemes in the Green's-functions approach, and the MF theory itself. It was shown that for all these theories the relevant information can be presented most compactly by considering the moments' generating function

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

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

$$M_1(x)=SB_S(xS)\ , \tag{7}$$

where

$$B_S(y)=\alpha\coth(\alpha\cdot y)-\beta\coth(\beta\cdot y) \qquad \left[\alpha=\frac{2S+1}{2S}\ ,\beta=\frac{1}{2S}\right] \tag{8}$$

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

$$x=\ln\left[1+\frac{1}{\Phi}\right] \tag{9}$$

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

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

$\epsilon_{\mathbf{p}}$ 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

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

[cf. Eq. (9)] and on knowledge of the algebraic connection between M_1 and Φ for all values of S which has been shown to be independent of the specific type of decoupling.[6,13,14] Now then, any moment is calculated from the generating function by simple differentiation:

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

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

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

and, consequently,

$$M_n=M_n\left[\frac{1}{S}B_S^{-1}(m)\right]\ . \tag{14}$$

C. The anisotropy coefficients as functions of magnetization

For the inversion of the Brillouin function [Eqs. (13) and (14)], an analytical method for S up to $\frac{3}{2}$,[18,19] and a parametric solution[3,11] for arbitrary spin has been invented. This parametric approach 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.[3] The most straightforward and effective way is to use as a parameter *the generalized effective fixed x itself.* It is so much the better that this parameter has a clear physical meaning, thus resembling the entropy difference parametrization of Lekner in a parametrical solution relevant to the critical point of a liquid.[20] 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 $T\rightarrow T_C$ 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_4 from Eq. (5) by using $M_2(x)$ and $M_4(x)$ from Eq. (12). Finally, collect pairs of computed points, corresponding to the same value of x, to plot or tabulate κ_4 as a function of magnetization. The curves $\kappa_4(m)$ obtained in this way for different values of S are universal for the whole class of theories as defined in Ref. 4.

Thus the general part of the analysis is now complete. At the same time, this section presented a concise account of the relevant notions and results which are preliminary to the new developments with which we now go ahead.

III. THE THEORETICAL FRAMEWORK: ITS PARTICULAR PART

The discussion is no longer valid for the whole class of Ref. 1 when one attempts to determine the *temperature* dependence of the anisotropy coefficients. One generic possibility which was put forward already in the pioneering paper by Wolf[5] is semiempirical and, in fact, sample specific. Namely, one inserts the dependence $m(T)$ as measured in experiment on the same sample and determines $\kappa_l(T)$. The other option is multifold and challenging: $m(T)$ has to be calculated within some theory from among the class of collective-excitations theories.

A. The MF temperature dependence of anisotropy

In the context of the outlined parametric approach, it is possible to determine quite easily the temperature dependence of the required quantities whenever the "tem-

perature part" in the generalized effective field x can be separated (factorized out) from the rest, i.e., from the magnetization and external field dependence.[21] Not unexpectedly, this separation is straightforward only for the MF theory of ferromagnetism which also belongs to the Callen and Shtrikman class. There,

$$x=\frac{3}{S+1}\cdot\frac{m}{t}\ , \tag{15}$$

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

$$t=t(x)=\frac{3}{S+1}\cdot\frac{m(x)}{x} \tag{16}$$

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. 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 in Refs. 3 and 11. This observation reflects back to those problems whose treatment was suggested in the last two papers. Note that as long as one works in the MF approximation the parametric solution for the temperature dependence of anisotropy has an explicit, analytic alternative for values of $S\leq\frac{3}{2}$ in lattice symmetry lower than cubic.[3]

B. The RPA temperature dependence of anisotropy for the fcc lattice

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.[15,7] Note that the geometry of the surroundings of a given spin is only very roughly accounted for in the MF approximation: in fact, it enters the theory only as the number of nearest neighbors to which the MF Curie temperature is proportional. This is quite unlike the RPA treatment where the energy spectrum of the quasiparticles is strongly dependent on the precise geometrical ordering [see Eqs. (17)–(19) below].

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).

The proposed parametric approach is certainly one of two new ingredients whose implementation makes possible the breakthrough beyond the MF temperature dependence of magnetic anisotropy. It will be seen in the following that this method makes it possible to circumvent solving the self-consistent Eq. (7) for the magnetization. In the RPA theory, this equation involves the triple sum Φ from Eq. (20) which depends on the magnetization because of the renormalization of the quasiparticle energy spectrum [Eqs. (17) and (27)]. The situation is much more complicated than in the MF case where the self-consistent equation is just a usual transcendental one. Note that it is not only the temperature dependence of anisotropy within the RPA which is entirely new: to our knowledge, the temperature dependence of the *magnetization itself* has not been reported for values of $S>\frac{1}{2}$, where the relation between Φ and m is nontrivial in contrast to the case with $S=\frac{1}{2}$.

The second, even more important ingredient is the calculation of the average occupation number of quasiparticle excitations Φ within the RPA. A method for the calculation of Φ valid for *any* type of lattice was proposed very recently.[10] 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 labor involved in cubic symmetry at least.

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

$$Q:\ \epsilon(\mathbf{k})/k_BT\equiv 2Q(1-\gamma_{\mathbf{k}})\ \ (0\leq Q\leq\infty)\ , \tag{17}$$

where the dispersion is determined by

$$\gamma_{\mathbf{k}}=J(\mathbf{k})/J(0)\ , \tag{18}$$

and

$$J(\mathbf{k})=\sum_{\mathbf{R}_{nn}}J(\mathbf{R})\exp(i\mathbf{k}\cdot\mathbf{R}) \tag{19}$$

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

$$\Phi(Q)=\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\exp[2Q(1-\gamma_{\mathbf{k}})]-1} \tag{20}$$

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,[10] here we give only the relevant final results. One finds that

$$\Phi(Q)_{|\mathrm{fcc}}=\Phi_0+\frac{1}{2}\sum_{k=1}^{\infty}(-1)^kA_k\frac{Q^k}{k!}\frac{d^k}{dQ^k}(\coth Q)\ , \tag{21}$$

where

$$\Phi_0=\frac{1}{\exp(2Q)-1} \tag{22}$$

and the coefficients A_k are defined via the triple trigonometric integrals

$$A_k(\text{fcc})=\frac{1}{\pi^3}\frac{1}{3^k}\int\int\int_0^{\pi}dx_1dx_2dx_3 \times(\cos x_1\cos x_2+\cos x_2\cos x_3+\cos x_3\cos x_1)^k . \quad (23)$$

A special procedure was developed for the calculation of the A_k's.[10] They can be found from

$$A_k=\sum_{q=0}^{k}c_{k-q}c_q \quad (24)$$

with the c_n's calculated from the three-position recursion relation[22]

$$c_{n+1}=\frac{n}{6(n+1)^2}[(4n+1)c_n+(2n-1)c_{n-1}] . \quad (25)$$

The required sum $\Phi(Q)$ is thus completely specified by the convergent expansion (21) supplemented with Eqs. (24) and (25) 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.[4] Furthermore, the same argument allows to interpret physically the parameter Q ($0\le Q\le\infty$). Namely, on comparing the expression

$$\Phi=\frac{1}{\exp(x)-1} , \quad (26)$$

which follows from Eq. (9) with Φ_0 from Eq. (22), 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 (21) 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 still fairly general. In fact, it is still valid for all but the trivial (MF) member of the class under consideration. The reason is that we introduced, intentionally, the flowing parameter Q quite formally by Eq. (17). 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 scheme.

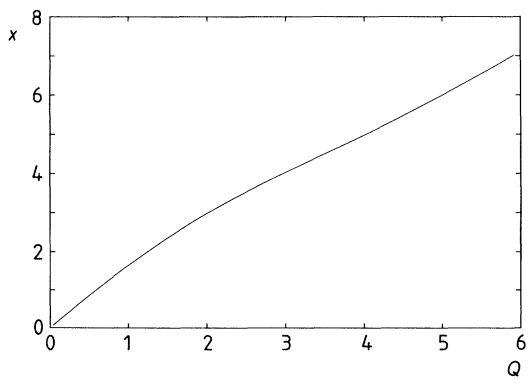

FIG. 1. Connection between the generalized effective field x and the flowing parameter Q. The dependence is linear only in the MF regime near the origin (small Q, $T\to T_C$), where $x=2Q$ (see text).

Comparing our formal definition of Q [Eq. (17)] with the renormalized energy spectrum in the RPA approximation,[12,7] we find

$$Q=\frac{3P(1)}{2S(S+1)}\cdot\frac{\langle S^z\rangle}{t}=\frac{3P(1)}{2(S+1)}\cdot\frac{m}{t} , \quad (27)$$

where m and t are, as above, the reduced magnetization and temperature and $P(1)=1.344\,66$ is the Watson integral for the fcc lattice.[23] 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[12,24] and is $P(1)$ times lower than the respective MF critical temperature. Solving Eq. (27) for t, one gets

$$t=t(Q)=\frac{3P(1)}{2(S+1)}\cdot\frac{m(Q)}{Q} . \quad (28)$$

The last equation completes the scheme for the implementation of the parametric method described in the previous subsection, 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

$$\Phi=\Phi(Q) , \quad (29)$$

$$M_n=M_n[x(\Phi(Q))]=M_n(Q) , \quad (30)$$

$$\kappa_l=\kappa_l\{M_n[x(\Phi(Q))]\}=\kappa_l(Q) , \quad (31)$$

$$t=t(m(Q),Q)=t(Q) . \quad (32)$$

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, $\Phi(t)$, etc.

IV. 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 made clear that one must specify the order in k in Eq. (21), up to which the summa-

tion for $\Phi(Q)$ has been carried out. Below, we report results up to and including $k=6$. There is no problem in carrying out the numerical computations to *any* k, because all quantities are easily calculable following work by Millev and Fähnle[10] [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, in Ref. 25]. The sum for $\Phi(Q)$ is convergent fast enough except at very low temperatures (large Q). Working up to $k=6$ gives for sufficiently low temperatures ($Q\approx 5$) average number of magnons of the order of 10^{-3}, which is the order of magnitude found in the asymptotically exact theory[26] (to leading order in $t=T/T_C$, both the RPA and Dyson's theory give the famous Bloch $T^{3/2}$ law.[27]) We thus conclude that for any practical purposes the order in k we considered provides for sufficient accuracy at all temperatures below T_c.

First, in Fig. 2 we give the temperature dependence, in reduced units, of the magnetization $m(T)$ in the RPA for all S between $\frac{1}{2}$ and $\frac{7}{2}$. Any other S can be just as easily calculated. We believe that already these results are not known for $S>\frac{1}{2}$. 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 orders 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 $S=2$, $\frac{5}{2}$, 3, $\frac{7}{2}$ (Fig. 4), which are 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, $S=\frac{5}{2}$. 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 for $T\to T_C$ which is not unexpected since the underlying asymptotic temperature dependences of the magnetization as $T\to T_C$ are identical and exhibit the MF critical exponent $\beta=\frac{1}{2}$. 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 anisot-

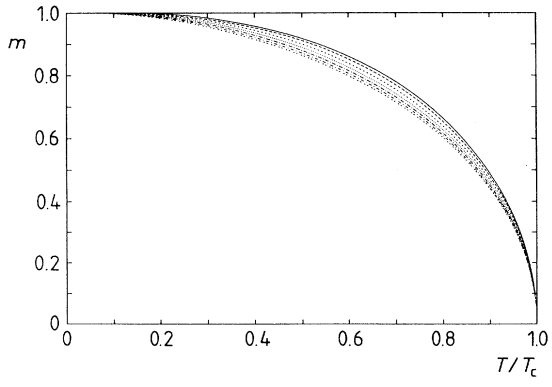

FIG. 2. Temperature dependence of the magnetization $m(T)$ in the RPA. The curves from above correspond to spins $\frac{1}{2}$–$\frac{7}{2}$. The curves for $S>\frac{1}{2}$ are reported for the first time. Note that our method does not evoke solution of integral expressions.

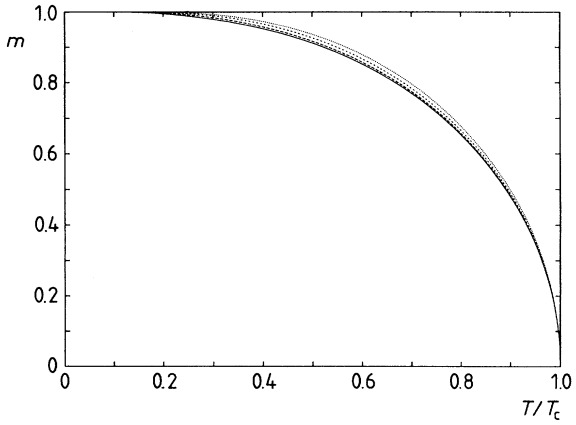

FIG. 3. The effect of orders in k on the temperature dependence of magnetization: curves from below correspond to $k=6$, 4, 2, and 0, resp. The highest curve is the MF prediction.

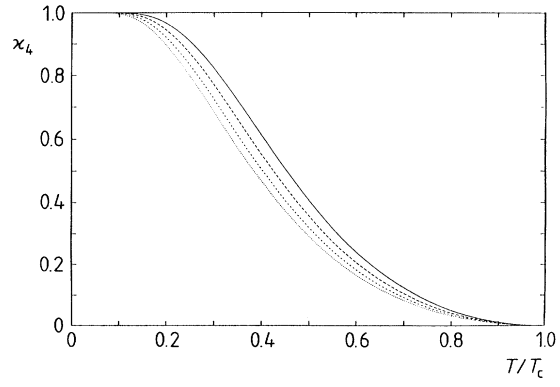

FIG. 4. MF temperature dependence of the first nonvanishing anisotropy coefficient $\kappa_4(T)$ curves from above correspond to $S=2$, $\frac{5}{2}$, 3, and $\frac{7}{2}$, resp.

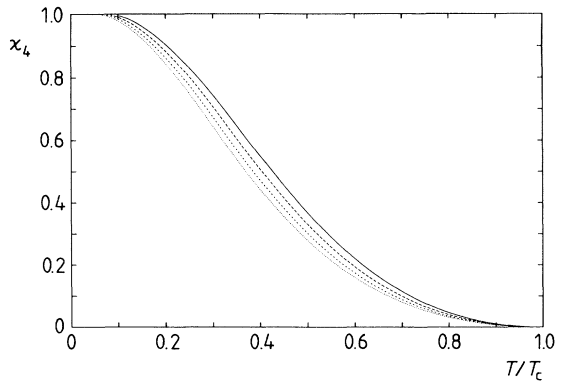

FIG. 5. RPA prediction for $\kappa_4(T)$. The curves are arranged as in Fig. 4. Note the bell shape and the fact that anisotropy curves even for neighboring spin values lie quite distinctly apart despite the proximity of the corresponding magnetization curves $m(T)$ (see Fig. 2).

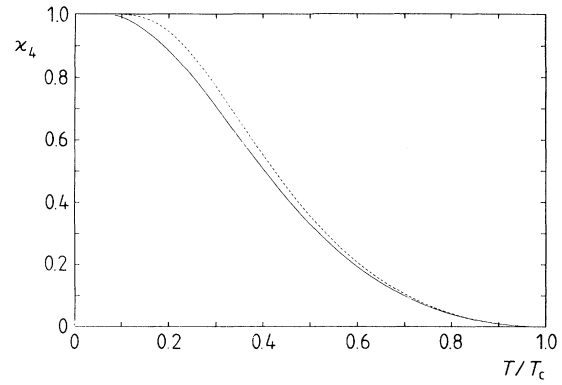

FIG. 6. Comparison of $\kappa_4(T)$ within MF and RPA: $S=\frac{5}{2}$. MF overestimates the anisotropy, and especially so at low temperatures. Both approximations converge for $T \rightarrow T_C$.

ropy in cubic materials has the peculiar bell shape, the bells being pronouncedly "slimmer" in the RPA as explained above. More precisely, in contrast to the first nontrivial anisotropy coefficient κ_2 in *noncubic* crystalline materials whose temperature dependence has been shown to be convex upwards for all T below T_C,[3] in *cubic* materials the respective curves for the first nontrivial anisotropy coefficient κ_4 do have an inflexion point approximately half way down from the Curie temperature. Strictly speaking, the last statement concerning cubic symmetry is proved here for all types of cubic lattice within the MF theory which is insensitive to fine structural details (cf. the first paragraph of Sec. III B and Fig. 4) and for the fcc lattice in the RPA. It seems reasonable to expect that the bell-shape feature persists in sc and bcc lattices as well.

Because the anisotropy coefficient κ_4 enters the leading anisotropy constant K_1 in cubic materials, an inflexion point in $\kappa_4(T)$ is consistent with an inflexion point in $K_1(T)$. It must be noted that qualitatively similar dependences for the anisotropy *constants* have recently been measured in novel hard magnetic materials like $R_2Fe_{17}N_x$ and $Sm_2Fe_{17}C_{3-\delta}$, though in symmetry lower than cubic.[28–30] The underlying reason for this similarity might be quite general and, possibly, independent of the type (soft or hard) of the magnetic material. In the above materials the first nonvanishing anisotropy coefficients entering the anisotropy constants are $\kappa_2(T)$ and $\kappa_4(T)$. Although $\kappa_2(T)$ is convex upwards for all T (see above), a bell shape of $K_1(T)$ may arise from the temperature dependence of $\kappa_4(T)$. This is presently being investigated within the framework of the mean-field approach.

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*On leave from the Institute of Applied Physics, Technical University, 1756 Sofia, Bulgaria.

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