pendence of nuclear cross sections is much larger. This difference tends to increase when one performs the average over $P(i,A)$ instead of the substitution $A^{1/3}$ in Eqs. (2)–(4).

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Comment on the Two-Ion Anisotropy in the Heavy-Rare-Earth Metals*

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The importance of anisotropic two-ion couplings in the rare-earth metals, Er and Tb, as deduced from measurements of the spin-wave energies, has recently been questioned by Lindgård. I find that this objection is based on an improper expansion of the excitation energies, and that the q-dependent single-ion contributions to the spin-wave energies are unimportant within a self-consistent Hartree-Fock approximation.

In a recent Letter,[1] Lindgård suggests that those effects observed in the spin-wave systems $Er^{2,3}$ and Tb,[4] which have been attributed to the presence of two-ion anisotropy, might be of single-ion origin. I shall present an analysis of the method used by Lindgård which shows that the modification of the spin-wave energies obtained is produced by an improper expansion of these energies. In order to illuminate the procedure of Lindgård I shall discuss mostly the simplest case of a planar ferromagnet,[5] which is qualitatively similar to the case of the conical ordered structure.

The Hamiltonian for the planar ferromagnet reads

$$\mathcal{H} = \sum_i (DJ_{x,i}^2 - g\mu_B H J_{z,i}) - \sum_{i,j} \mathcal{J}(i,j)\vec{J}_i \cdot \vec{J}_j. \tag{1}$$

$\vec{J}_i$ is the total angular moment of the ith ion, D is positive, and H is a field applied along the direction of magnetization (z direction). When the moments are close to their maximum value, $\langle J_{z,i} \rangle \cong J$, the normal procedure is to introduce spin-deviation operators by the Holstein-Primakoff transformation followed by a Fourier transformation:

$$\mathcal{H} = JN[\tfrac{1}{2}D - g\mu_B H - J\mathcal{J}(0)] + \sum_{\vec{q}} [A_{\vec{q}} a_{\vec{q}}^\dagger a_{\vec{q}} + \tfrac{1}{2}B_{\vec{q}}(a_{\vec{q}}^\dagger a_{-\vec{q}}^\dagger + a_{\vec{q}} a_{-\vec{q}})] + \ldots , \tag{2}$$

where terms involving products of more than two spin-deviation operators are not explicitly shown. They may be taken into account, approximately, by a self-consistent Hartree-Fock calculation. In this case the energy of the (undamped) elementary excitations is temperature dependent[6,7]:

$$E_{\vec{q}}(T) = \{[A_{\vec{q}}(T) + B_{\vec{q}}(T)][A_{\vec{q}}(T) - B_{\vec{q}}(T)]\}^{1/2}, \tag{3}$$

where

$$A_{\vec{q}}(T) = 2J[\mathcal{J}(0) - \mathcal{J}(\vec{q})](1 - m) + g\mu_B H + D(J - \tfrac{1}{2})(1 - 2m - b) + \sum_{\vec{k}} 2J[\mathcal{J}(\vec{k}) - \mathcal{J}(\vec{k} - \vec{q})]m_{\vec{k}} \tag{4a}$$

and

$$B_{\vec{q}}(T) = D(J - \tfrac{1}{2})(1 - 2m - b) + \sum_{\vec{k}} 2J[\mathcal{J}(\vec{k}) - \mathcal{J}(\vec{k} - \vec{q})]b_{\vec{k}} \tag{4b}$$

when including the terms of first order in $1/J$, which is the order of the temperature-dependent parameters $m_{\vec{k}}$ and $b_{\vec{k}}$. These parameters are determined self-consistently by

$$m = N^{-1}\sum_{\vec{k}} m_{\vec{k}}, \quad m_{\vec{k}} = J^{-1}(\{n[E_{\vec{k}}(T)] + \tfrac{1}{2}\}A_{\vec{k}}(T)/E_{\vec{k}}(T) - \tfrac{1}{2}),$$

$$b = N^{-1}\sum_{\vec{k}} b_{\vec{k}}, \quad b_{\vec{k}} = -J^{-1}\{n[E_{\vec{k}}(T)] + \tfrac{1}{2}\}B_{\vec{k}}(T)/E_{\vec{k}}(T), \tag{5}$$

where $n(E)$ is the boson population factor. The energy of the uniform mode, $E_{\vec{q}=0}(T)$, is zero in accordance with the Goldstone theorem, which is violated (in the order J^{-1}) if the last term of (2) is neglected (see the discussion by Jensen[7]). The higher-order terms in m and b may be of some importance for determining the renormalized values of the crystal-field parameters of high ranks. A reasonable way of

accounting for these terms is to interpret the first-order terms appearing in (4) as being produced by power-law expressions like $(1 - m)^{\alpha}(1 - b)^{\beta}$; see, for instance, Ref. 7.

In this theory two approximations are made. Only the matrix elements of the Hamiltonian between the three J_z wave functions, $|J\rangle$, $|J - 1\rangle$, and $|J - 2\rangle$, are treated correctly; however, these states are the most important ones in the case of a spin-wave system; furthermore, the other matrix elements deviate only in the order $1/J^2$ and are effectively included above the power-law generalization. The other approximation is the Hartree-Fock (or random-phase) decoupling of the higher-order terms. When m and b are small (low temperatures) this approximation should not lead to a change of the results by an order of magnitude.

In his recent Letter[1,5] Lindgård makes use of the wave functions diagonalizing (approximately) the molecular-field Hamiltonian as basis instead of the J_z wave functions. In order to perform the diagonalization, $e = D(J - \tfrac{1}{2})/[2J\mathcal{I}(0) + g\mu_B H]$ is utilized as an expansion parameter. Introducing boson operators annihilating (or creating) the molecular-field excitations, these new operators, $a_i{}^*$, may be obtained from the spin deviation operators by a unitary transformation.

In terms of the new operators the Hamiltonian may be written in a way similar to (2), replacing $A_{\vec{q}}$ and $B_{\vec{q}}$ by $A_{\vec{q}}{}^{\mathrm{MF}}$ and $B_{\vec{q}}{}^{\mathrm{MF}}$. The higher-order terms are changed so that the molecular-field Hamiltonian contributes only with terms that are diagonal in the new operators [e.g., $(a_i{}^* a_i{}^*)^\dagger a_i{}^* a_i{}^*$], implying that a number of the higher-order terms are included exactly in $A_{\vec{q}}{}^{\mathrm{MF}}$ and $B_{\vec{q}}{}^{\mathrm{MF}}$. A few considerations show that the terms which are included are those corresponding to the molecular-field values of m and b

$$m_0 = (4J)^{-1}e^2(1 - 2e) + O(e^4), \quad b_0 = -(2J)^{-1}e(1 - e) + O(e^3),\qquad(6)$$

at zero temperature. A straightforward calculation of the molecular-field parameters gives at zero field

$$A_{\vec{q}}{}^{\mathrm{MF}} = 2J[\mathcal{I}(0) - \mathcal{I}(\vec{q})] + D(J - \tfrac{1}{2}) - \frac{D^2(J - \tfrac{1}{2})(J - 1)}{4J\mathcal{I}(0)}\left[1 + \frac{\mathcal{I}(\vec{q})}{\mathcal{I}(0)}\right]$$

$$+ \frac{D^3(J - \tfrac{1}{2})(J - 1)}{8J^2\mathcal{I}^2(0)}\left[(J - 2) + 2(J - 1)\frac{\mathcal{I}(\vec{q})}{\mathcal{I}(0)}\right] + O(e^4)\qquad(7a)$$

and

$$B_{\vec{q}}{}^{\mathrm{MF}} = D(J - \tfrac{1}{2})\left[1 - \frac{D(J - 1)}{2J\mathcal{I}(0)}\right]\frac{\mathcal{I}(\vec{q})}{\mathcal{I}(0)} + O(e^3).\qquad(7b)$$

Introducing (7) into (3) and neglecting terms of the order e^{α}/J^2, $\alpha = 1,2,3$, corresponding to b/J and m/J, we get

$$E_{\vec{q}}{}^2 = 2J[\mathcal{I}(0) - \mathcal{I}(\vec{q})]\left(1 - \frac{e^2}{4J} + \frac{e^3}{2J}\right)\left\{2J[\mathcal{I}(0) - \mathcal{I}(\vec{q})]\left(1 - \frac{e^2}{4J} + \frac{e^3}{2J}\right) + 2D(J - \tfrac{1}{2})\left(1 + \frac{e}{2J} - \frac{e^2}{J}\right)\right\} + O(e^4)\qquad(8a)$$

which agrees with that obtained from (4) introducing the values m_0 and b_0 for m and b. In order to calculate the field dependence of $E_{\vec{q}}{}^2$ one has to take into account that e and thus both $A_{\vec{q}}{}^{\mathrm{MF}}$ and $B_{\vec{q}}{}^{\mathrm{MF}}$ are field dependent. In the molecular-field approach the result is

$$\lim_{H \to 0}\frac{d}{dH}E_{\vec{q}}{}^2 = 2g\mu_B\left\{2J[\mathcal{I}(0) - \mathcal{I}(\vec{q})]\left(1 - \frac{e^2}{4J} + \frac{e^3}{2J}\right) + D(J - \tfrac{1}{2})\left(1 + \frac{e}{2J} - \frac{e^2}{J}\right)\right.$$

$$\left. - \tfrac{1}{2}De(1 - \gamma_{\vec{q}})[\gamma_{\vec{q}} - e(3\gamma_{\vec{q}} + 2)] + O(e^4)\right\};\qquad(8b)$$

$\gamma_{\vec{q}}$ is $\mathcal{I}(\vec{q})/\mathcal{I}(0)$. This result is identical to the one obtained in the spin-wave theory (the last term is due to the field dependence of m_0 and b_0). Accounting for the terms of zero and first order in $1/J$ the two theories agree at least to third order in e. The comparison supports very strongly our assertion that the Hartree-Fock approximation should not introduce errors changing the results by an order of magnitude. This implies that to zero order in $1/J$ the two theories should agree to all orders in e, as the zeroth-order theory neglects the higher-order terms in (2) making the spin waves into perfect har-

monic oscillators. In fact, the close agreement obtained above indicates that the Hartree-Fock decoupling of the $1/J$ terms eventually may introduce errors only in the order $1/J^2$.

The case of a conical ordered structure does not introduce any essential differences. The modification of the spin-wave energies of the cone, which is considered by Lindgård,[1] is of zeroth order in $1/J$. Proceeding as above we find in this order of $1/J$

$$A_{\vec{q}}^{\mathrm{MF}} = H_{\mathrm{ex}} + D_0 - \Delta_{\vec{q}} - A_{\vec{q}}^{\mathrm{ex}} + B_q^{\mathrm{ex}} D_2/H_{\mathrm{ex}} - \tfrac{1}{2}(H_{\mathrm{ex}} + A_{\vec{q}}^{\mathrm{ex}} + 2B_{\vec{q}}^{\mathrm{ex}} D_0/D_2)(D_2/H_{\mathrm{ex}})^2 + O(e^3) \tag{9a}$$

and

$$B_{\vec{q}}^{\mathrm{MF}} = -B_{\vec{q}}^{\mathrm{ex}} + A_{\vec{q}}^{\mathrm{ex}} D_2/H_{\mathrm{ex}} - \tfrac{1}{2}(B_{\vec{q}}^{\mathrm{ex}} + 2A_{\vec{q}}^{\mathrm{ex}} D_0/D_2)(D_2/H_{\mathrm{ex}})^2 + O(e^3) \tag{9b}$$

$(e = D_2/H_{\mathrm{ex}})$. If the second-order terms are neglected, these are the expressions used by Lindgård in his analysis of the spin waves in Er (the notation is the one used in his paper). However, a consistent calculation of the spin-wave energies to either first or second order in e agrees with with the result obtained using the J_z wave functions as basis (the alteration introduced by Lindgård is of second order in e and disappears when all second-order terms are included). I shall add that e is not a legitimate expansion parameter in the case of Er because it is larger than 1. This has no serious consequences for the spin-wave theory (as long as m and b are still small, which is the case in Er), but the diagonalization of the molecular-field Hamiltonian has to be performed in another way (utilizing $1/J$ as an expansion parameter). A numerical calculation in the case of Er gave a very satisfactory agreement between the two theories (i.e., by adjusting the constant spin-wave parameter,[3] L, the dispersion relations agreed within a few percent). The equivalence of the two theories (as also indicated by a $1/J$ expansion of the molecular-field Hamiltonian) is easily obtained using the formulation of the following Comment by Lindgård.[8] If those higher-order spin terms ⌊in his Eq. (5)⌋ which couple the ground state and the third and higher-lying levels are neglected then $\langle 0 |[\tilde{S}^+, \tilde{S}^-] |0 \rangle/(2S)$ $= 1 - m$ is equal to $(1+\alpha)^2 - \beta^2 = (1+\epsilon)(1 - \beta_\chi^2)^{1/2}$ which immediately reduces $(E_q^{\mathrm{MME}})^2$ ⌊in his Eq. (8)⌋ to the spin-wave expression ⌊in the cone phase, Δ_g is also multiplied by $(1+\epsilon)(1 - \beta_\chi^2)^{1/2}$⌋.

The renormalization of the spin-wave parameters is of importance only when e is of the order of 1. In order to make sure that the terms of higher ranks (which contribute significantly in the order $1/J^2$) do not alter the results essentially, we made an exact numerical analysis of a specific example corresponding to Tb (for $e \cong 0.38$). A very convincing agreement between the two theories was found. The only discrepancy detected was in the values of the renormalized single-ion parameters (B_{60} and B_{66} are changed as much as by 50%). However, when the renormalized values of these parameters were adjusted (e.g., by introducing a 30% larger effective value of b), the dispersion of the excitations agreed within one to two parts in a thousand, both at zero and at finite fields, implying that the renormalization of the two-ion contribution differs slightly from $1 - m$. This difference, being of the order of b^2 or b/J, is one order-of-magnitude smaller than the random-phase contributions [the last terms of (4a) and (4b)].

The molecular-field approach gives results which agree qualitatively with the spin-wave theory. The Hartree-Fock decoupling of the higher-order single-ion terms seems to introduce errors only in the order $1/J^2$. The spin-wave theory has not been carried out to this order; however, the generalized power-law expressions account for about 80% of the renormalization of the crystal-field parameters (in this numerical example). The intermediate parameters $A_{\vec{q}}$ and $B_{\vec{q}}$ are transformed when we change the basis wave functions. In the hybridized molecular-field–random-phase approximation used above, this transformation does not affect the excitation energies to zeroth or first order in $1/J$. The changes of $A_{\vec{q}}$ and $B_{\vec{q}}$ are required if the two theories should compare also when including the differences between the molecular-field and random-phase values of m and b. Molecular-field correction parameters, m^{MF} and b^{MF} ⌊obtained from (5) when replacing $A_{\vec{q}}$ and $B_{\vec{q}}$ by $A_{\vec{q}}^{\mathrm{MF}}$ and $B_{\vec{q}}^{\mathrm{MF}}$⌋ appear in (7) in a way similar to how m and b occur in (4). In the ferromagnet, $B_{\vec{q}}^{\mathrm{MF}}$ is proportional to $\mathcal{J}(\vec{q})$ [a $\vec{q}$ dependence which does not compare with $B(\vec{q})$ determined in Tb by Jensen, Houmann, and Møller[4]] which allows the identification of the m and b values, (6), to be used when m^{MF} and b^{MF} are both zero. We shall add that the $\vec{q}$ dependence of $B_{\vec{q}}^{\mathrm{MF}}$ implies that b^{MF} will normally be an order of magnitude smaller than b, indicating that the molecular-field wave functions provide a better basis than the J_z wave functions (assuming

an accurate treatment of the molecular-field Hamiltonian).

This analysis allows one to place confidence in the genuine $\bar{q}$-dependent single-ion contributions deduced in the Hartree-Fock approximation. The $B(\bar{q})$ deduced in Tb from the field dependence of the spin-wave energies[4] corresponds to $B_{\bar{q}}$, (4b); and the $\bar{q}$-dependent single-ion contribution to this term is, at least, smaller than $|2J\mathcal{J}(0)b| \approx 0.25$ meV, which is negligible in comparison with the actual $\bar{q}$ dependence. A similar estimate in the case of Er shows that the single-ion contribution to the dispersive terms is of the order of 0.1 meV, which is much less than the effective two-ion anisotropy[3] deduced to be of the order of 1 meV. In conclusion, I consider the abnormal dispersive effects observed in Tb and Er, being at least an order of magnitude larger than those originating from the single-ion terms, to be clear evidences for the presence of the anisotropic two-ion couplings in these metals.

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Reply to Comment on the Two-Ion Anisotropy in the Heavy-Rare-Earth Metals

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The giant anisotropic two-ion couplings found in Er and Tb do not break the symmetry of the lattice. A nonspherical spin pressession due to crystal field effects was recently shown to induce such couplings from a basically isotropic interaction. The argument is here shown to be generally valid. It is shown that the conventional theory combined with the Hartree Fock approximation underestimates the effect of such ground-state corrections.

It was recently argued[1] that the conventional spin-wave theory does not treat the anisotropy adequately in strongly anisotropic systems. A systematic perturbation approach in $V_c/H_{ex}S$, the crystal-field energy V_c versus the exchange-field energy $H_{ex}S$, was proposed and shown to provide a possible explanation for the apparent giant two-ion anisotropy in the heavy-rare-earth metals. The first-order boson theory[1] was subsequently generalized to an infinite-order spin formalism[2] and it was shown that, for simple reasons, the first-order spin-wave expression assumes the most general form to which spin waves can be fitted, provided the parameters are interpreted as being renormalized. Since the relevant spin excitation operators are obtained by the matching of matrix element (MME) method, this theory is called the MME theory. In the preced-

ing Comment,[3] Jensen agrees that this theory [somewhat misleadingly denoted as a molecular-field (MF) theory] is correct and normally an order of magnitude more accurate with respect to the ground-state corrections than the conventional theory. Nevertheless, Jensen attempts to argue that (more) reliable results might be obtained on the basis of the conventional theory, treating some of the higher-order terms (of order $1/J$) in the Hartree-Fock (HF) approximation. The arguments presented[3] are incorrect and misleading as will be demonstrated below.

Consider the simple example of a nearest-neighbor ferromagnet with planar anisotropy at $T = 0$. The notation is the same as used in the preceding Comment by Jensen[3] [and references to his equations will be denoted by J]. The spin-wave functions in the conventional (CHF) theory