

# Uniform spin wave modes in antiferromagnetic nanoparticles with uncompensated moments

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**Abstract.** In magnetic nanoparticles the uniform precession ( $\mathbf{q} = 0$  spin wave) mode gives the predominant contribution to the magnetic excitations. We have calculated the energy of the uniform mode in antiferromagnetic nanoparticles with uncompensated magnetic moments, using the coherent potential approximation. In the presence of uncompensated moments, an antiferromagnetic nanoparticle must be considered as a kind of a ferrimagnet. Two magnetic anisotropy terms are considered, a planar term confining the spins to the basal plane, and an axial term determining an easy axis in this plane. Excitation energies are calculated for various combinations of these two anisotropy terms, ranging from the simple uniaxial case to the planar case with a strong out-of-plane anisotropy. In the simple uniaxial case, the uncompensated moment has a large influence on the excitation energy, but in the planar case it is much less important. The calculations explain recent neutron scattering measurements on nanoparticles of antiferromagnetic  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and NiO.

**PACS.** 76.50.+g Ferromagnetic, antiferromagnetic, and ferrimagnetic resonances; spin-wave resonance – 75.75.+a Magnetic properties of nanostructures – 75.50.Ee Antiferromagnetics – 75.30.Gw Magnetic anisotropy

## 1 Introduction

The magnetic properties of nanoparticles have been the subject of numerous studies, partly because of the many technological applications of magnetic nanoparticles [1,2]. Several experimental and theoretical studies of spin waves in low-dimensional systems have been published [3–7]. In magnetic nanoparticles, it is characteristic that the magnetisation direction is not fixed as in bulk materials, but fluctuates due to thermal excitation of the uniform precession mode. Such uniform precession around an easy direction of magnetisation in combination with transitions between precession states with different precession angles have been termed collective magnetic excitations [8,9]. As the temperature is increased such that the magnetic anisotropy energy is comparable to the thermal energy, the fluctuations become dominated by superparamagnetic relaxation, i.e. thermally induced magnetisation reversals.

The uniform precession states are predominant in nanoparticles compared to other spin wave excitations [10] and these precession states can be described as spin waves with the wave vector  $\mathbf{q} = 0$ . Uniform excitations in

bulk antiferromagnetic materials are conventionally studied by antiferromagnetic resonance (AFMR) experiments, see, for example [11]. However, only few magnetic resonance studies have been performed on antiferromagnetic nanoparticles [12,13].

Inelastic neutron scattering has been shown to be a useful tool for measuring the excitation energy of the uniform precession states [14]. The quantised nature of the  $\mathbf{q} = 0$  spin waves and also the polarisation of these may be studied by this method [15].

Many previous calculations concerning antiferromagnetic spin waves assume a uniaxial anisotropy described by a single anisotropy term [16]. However, often the anisotropy is better described by more than one term. In the present paper the  $\mathbf{q} = 0$  spin wave energies in the presence of both a negative planar anisotropy energy  $\kappa_1$ , and a positive axial in-plane anisotropy energy  $\kappa_2$ , are calculated. This description is applicable e.g. to hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) and NiO. In both bulk materials the value of  $|\kappa_2|$  is very small compared to  $|\kappa_1|$ . In nanoparticles of these materials, the axial anisotropy energy has been found to be orders of magnitude larger than in bulk although still significantly smaller than the planar anisotropy energy [17,18]. This can be explained by the influence of

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surface anisotropy [19], which results from the low symmetry around the surface atoms.

In general, a nanoparticle of an antiferromagnetic material is not a perfect antiferromagnet, but has an uncompensated magnetic moment due to different numbers of spins in the two sublattices. This was proposed theoretically by Néel [20] and has been observed in nanoparticles of different antiferromagnetic materials such as ferritin [21,22] NiO [23–25], and Cr<sub>2</sub>O<sub>3</sub> [26].

In this paper, we use the coherent potential approximation to derive expressions for the energy of the uniform excitations in nanoparticles with uncompensated magnetic moments, and with axial and planar magnetic anisotropy terms, similar to those of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and NiO. We find that the effect of an uncompensated moment on the excitation energy depends strongly on the ratio between the two contributions to the anisotropy. The calculations assume localised spins, and neglect any non-collinear spin structures such as spin-canting. In real nanoparticles spin-canting may be present both at the surface and within the particles [27]. Our model may be generalized to include this.

## 2 Uniform mode spin waves in a finite lattice with planar and axial anisotropy

We consider a nanoparticle of a two-sublattice antiferromagnet with sublattice labels  $A$  and  $B$ . The number of magnetic ions on sublattice  $A$  is  $N_A$  and on sublattice  $B$  it is  $N_B$ . The index of sublattice  $A$  is  $j$ , and the index of sublattice  $B$  is  $l$ . The ratio between the number of spins on the sublattices is  $\xi = \frac{N_B}{N_A}$ . The uncompensated spin is defined as  $|s(N_A - N_B)| = |sN_A(1 - \xi)|$ .

The ground state of the system is assumed to be the Néel state with the spins on the sublattice  $A$  aligned along the positive  $z$  direction and those on sublattice  $B$  aligned along the negative  $z$  direction.

The Hamiltonian of the system with spins  $\mathbf{s}_j$  and  $\mathbf{s}_l$  can be written as

$$\mathcal{H} = \sum_{jl} J_{jl} \mathbf{s}_j \cdot \mathbf{s}_l - \left( \sum_j \kappa_{1j} (s_j^x)^2 + \sum_l \kappa_{1l} (s_l^x)^2 \right) - \left( \sum_j \kappa_{2j} (s_j^z)^2 + \sum_l \kappa_{2l} (s_l^z)^2 \right) \quad (1)$$

where  $J_{jl}$  are the inter-sublattice exchange constants,  $z$  is the easy axis of the spins within the easy plane and  $x$  is perpendicular to the easy plane. Choosing the anisotropy constants  $\kappa_{1j}$  and  $\kappa_{1l}$  negative and  $\kappa_{2j}$  and  $\kappa_{2l}$  positive we maintain a ground state with the spins pointing along  $z$ . For a nanoparticle the anisotropy depends on the site  $j, l$  because atoms near the surface may have an anisotropy that differs from that of atoms in the interior of the particles. For simplicity, we here assume that the anisotropy energy has the same form for all atoms. Since we will only consider the  $\mathbf{q} = 0$  spin wave mode, we may disregard the

intra-sublattice interaction, i.e. the  $J_{jj'}$  and  $J_{ll'}$ -terms in the Hamiltonian.

The initial calculations follow the procedure outlined by Marshall and Lovesey [28], but differ by not assuming translational symmetry. For completeness, we here sketch the full calculation leading to the final spin wave expression. The spin raising and lowering operators  $s^\pm = s^x \pm is^y$  satisfy the commutator relations

$$[s_n^+, s_m^-] = 2s_n^z \delta_{n,m} \quad \text{and} \quad [s_n^z, s_m^\pm] = \pm s_n^\pm \delta_{n,m} \quad (2)$$

where  $m$  and  $n$  refer to spins on either of the sublattices. Rotating the  $B$  sublattice by  $\pi$  about the  $x$  axis gives new operators,  $t$ , where

$$\begin{aligned} t_l^x &= s_l^x & t_l^y &= -s_l^y & t_l^z &= -s_l^z \\ t_l^+ &= s_l^- & t_l^- &= s_l^+ \end{aligned} \quad (3)$$

At low temperature the spins will predominantly be along  $z$  in one sublattice and along  $-z$  in the other sublattice, such that  $s_j^z \approx s$  and  $t_l^z \approx -s$  are valid approximations.

Including only linear terms we reach four equations of motion for individual spin site operators:

$$\begin{aligned} i\hbar \frac{d}{dt} s_j^\pm &= [s_j^\pm, \mathcal{H}] \\ &= \pm s \sum_l J_{jl} (s_j^\pm + t_l^\mp) + 2\kappa_{2j} s' s_j^\pm \\ &\quad - \kappa_{1j} s' (s_j^\pm + s_j^\mp) \end{aligned} \quad (4)$$

$$\begin{aligned} i\hbar \frac{d}{dt} t_l^\pm &= [t_l^\pm, \mathcal{H}] \\ &= \pm s \sum_j J_{jl} (t_l^\pm + s_j^\mp) + 2\kappa_{2l} s' t_l^\pm \\ &\quad - \kappa_{1l} s' (t_l^\pm + t_l^\mp). \end{aligned} \quad (5)$$

To obtain the correct quantum mechanical form for the anisotropy terms, we have used the well ordered Holstein-Primakoff transformation [29]. This gives the factor  $s' = s - \frac{1}{2}$  in the anisotropy terms, instead of the classical  $s$ .

The creation operator of a  $\mathbf{q} = 0$  spin wave is a linear combination of the four operators  $S^\pm = \sum_j s_j^\pm$  and  $T^\pm = \sum_l t_l^\pm$ . Using (4), (5) and a coherent potential approximation for the anisotropy terms, we reach the equations of motion for these:

$$\begin{aligned} i\hbar \frac{d}{dt} S^\pm &= [S^\pm, \mathcal{H}] \\ &= \pm s \sum_{jl} J_{jl} (t_l^\mp + s_j^\pm) \mp \kappa_1 s' (S^+ + S^-) \\ &\quad \pm \kappa_2 2s' S^\pm \end{aligned} \quad (6)$$

$$\begin{aligned} i\hbar \frac{d}{dt} T^\pm &= [T^\pm, \mathcal{H}] \\ &= \pm s \sum_{jl} J_{jl} (s_j^\mp + t_l^\pm) \mp \kappa_1 s' (T^+ + T^-) \\ &\quad \pm \kappa_2 2s' T^\pm, \end{aligned} \quad (7)$$

where the average anisotropy constants are

$$\kappa_n = \frac{1}{2} \left( \frac{\sum_j \kappa_{nj}}{N_A} + \frac{\sum_l \kappa_{nl}}{N_B} \right), \quad n = 1, 2. \quad (8)$$

To show that there are no terms missing from (6) and (7) although  $jj'$  and  $l'l$ -terms were left out of the Hamiltonian (1), consider the term in the double-sums,  $J_{jl}(t_l^\mp + s_j^\pm)$  and  $J_{jl}(s_j^\mp + t_l^\pm)$ . These terms are antisymmetric with respect to the indices, since  $s_l^\pm = \mp t_l^\mp$  and  $t_j^\pm = \mp s_j^\mp$ . If a term of index  $jj'$  appears in the same sum as one of index  $j'j$ , these will cancel out. Hence, we are left only with bonds connecting sites on opposite sublattices.

This enables us to easily count the total number of bonds on each sublattice, and we will now use this to approximate the double sums,

$$\sum_{jl} J_{jl}(t_l^\mp + s_j^\pm) \quad \text{and} \quad \sum_{jl} J_{jl}(s_j^\mp + t_l^\pm). \quad (9)$$

The method for infinite systems is to use periodic boundary conditions. However, this is invalid for nanoparticles. In our case, the number of bonds to a site varies, depending on the position in the nanoparticle.

Consider a specific nanoparticle. For simplicity, we assume that the interior of the nanoparticle is defect-free with  $Z_{\text{int}}$  bonds to each of the  $N_{\text{int}}$  internal sites. Suppose that on average, there are  $Z_{\text{surf}}$  bonds to each of the  $N_{\text{surf}}$  surface sites. The total number of bonds connecting sublattices  $A$  and  $B$  of a particular nanoparticle, is

$$K = Z_{\text{surf},A}N_{\text{surf},A} + Z_{\text{int},A}N_{\text{int},A} \quad (10)$$

$$= Z_{\text{surf},B}N_{\text{surf},B} + Z_{\text{int},B}N_{\text{int},B}. \quad (11)$$

However, the average number of bonds seen from either sublattice, differs. Notice that  $K$  depends on  $N_A$ ,  $N_B$ , and the shape of the particle.

We can now define the weighted average  $\mathcal{J}(0)_I^{\text{av}}$  =  $JZ_I^{\text{av}}$  for each sublattice, by

$$\mathcal{J}(0)_A^{\text{av}} = J \frac{Z_{\text{surf},A}N_{\text{surf},A} + Z_{\text{int},A}N_{\text{int},A}}{N_A} = \frac{JK}{N_A} \quad (12)$$

$$\mathcal{J}(0)_B^{\text{av}} = J \frac{Z_{\text{surf},B}N_{\text{surf},B} + Z_{\text{int},B}N_{\text{int},B}}{N_B} = \frac{JK}{N_B} \quad (13)$$

$$\mathcal{J}(0)_A^{\text{av}} = \xi \mathcal{J}(0)_B^{\text{av}}. \quad (14)$$

This is a coherent potential approximation for the exchange interaction. The microscopic approach allows us to treat the anisotropy and sublattice interaction in a quantum mechanically correct way.

We can now use the coherent potential and (12)–(14), to approximate (9):

$$\begin{aligned} \sum_{jl} J_{jl}(t_l^\mp + s_j^\pm) &= \mathcal{J}(0)_B^{\text{av}} \sum_l t_l^\mp + \mathcal{J}(0)_A^{\text{av}} \sum_j s_j^\pm \\ &= \mathcal{J}(0)_B^{\text{av}} T^\mp + \mathcal{J}(0)_A^{\text{av}} S^\pm \\ &= \mathcal{J}(0)_B^{\text{av}} (T^\mp + \xi S^\pm) \end{aligned} \quad (15)$$

$$\sum_{jl} J_{jl}(s_j^\mp + t_l^\pm) = \mathcal{J}(0)_B^{\text{av}} (\xi S^\mp + T^\pm). \quad (16)$$

This approximation is only valid in the case where  $\mathbf{q} = 0$ , because  $\mathcal{J}(\mathbf{q})$  contains intra-sublattice terms for  $\mathbf{q} \neq 0$ .

Using (15) and (16), the equations of motion (6) and (7) are readily solved. In matrix form, we have

$$\begin{bmatrix} \xi \mathcal{J}(0)^{\text{av}} s + a & b & 0 & \mathcal{J}(0)^{\text{av}} s \\ -b & -\xi \mathcal{J}(0)^{\text{av}} s - a & -\mathcal{J}(0)^{\text{av}} s & 0 \\ 0 & \xi \mathcal{J}(0)^{\text{av}} s & \mathcal{J}(0)^{\text{av}} s + a & b \\ -\xi \mathcal{J}(0)^{\text{av}} s & 0 & -b & -\mathcal{J}(0)^{\text{av}} s - a \end{bmatrix} \quad (17)$$

where  $a = (2\kappa_2 - \kappa_1)s'$ ,  $b = \kappa_1 s'$  and  $\mathcal{J}(0)^{\text{av}} = \mathcal{J}(0)_B^{\text{av}}$ . The eigenvalues of this matrix are the energies of the uniform modes.

## 2.1 Energies of the uniform mode

### 2.1.1 Perfect antiferromagnetic nanoparticle

In a perfect antiferromagnetic nanoparticle the number of spins is the same on both sublattices such that  $\xi = 1$ . Solving equation (17) gives the four solutions

$$\hbar\omega_\alpha = \pm 2\sqrt{\kappa_2 s' [(\kappa_2 - \kappa_1)s' + \mathcal{J}(0)^{\text{av}} s]} \quad (18)$$

$$\hbar\omega_\beta = \pm 2\sqrt{(\kappa_2 - \kappa_1)s' [\kappa_2 s' + \mathcal{J}(0)^{\text{av}} s]} \quad (19)$$

The anisotropy and exchange fields are defined as

$$B_{Ai} = \frac{2|\kappa_i|s'}{g\mu_B} \quad (i = 1, 2) \quad (20)$$

and

$$B_E = \frac{|\mathcal{J}(0)^{\text{av}}|s}{g\mu_B} = \frac{c}{g\mu_B}, \quad (21)$$

where  $g$  is the  $g$ -factor and  $\mu_B$  is the Bohr magneton.

Usually  $B_E \gg B_{Ai}$  and  $B_{A1} \gg B_{A2}$ . Thus ignoring the negative solutions the spin wave energies may be approximated by

$$\hbar\omega_\alpha \approx g\mu_B \sqrt{2B_{A2}B_E} \quad (22)$$

$$\begin{aligned} \hbar\omega_\beta &\approx g\mu_B \sqrt{2(B_{A2} + B_{A1})B_E} \\ &\approx g\mu_B \sqrt{2B_{A1}B_E}. \end{aligned} \quad (23)$$

The expressions are recognised as the conventional expressions for antiferromagnetic resonance [11].

### 2.1.2 Lattice with uncompensated moments

As proposed by Néel [20] the small size of an antiferromagnetic nanoparticle generally will result in an excess number of spins on one sublattice compared to the other, i.e.,  $\xi \neq 1$ . In this case the solutions to equation (17) become more complex. Using the symbols defined above and defining

$$d = \sqrt{4a^2(\xi - 1)^2 + c^2(\xi - 1)^4 + 16b^2\xi + 4ac(\xi - 1)^2(\xi + 1)} \quad (24)$$

the spin wave energies are given by

$$\hbar\omega_\alpha = \sqrt{a^2 - b^2 + ac(\xi + 1) + \frac{1}{2}c^2(\xi - 1)^2 - \frac{1}{2}cd} \quad (25)$$

$$\hbar\omega_\beta = \sqrt{a^2 - b^2 + ac(\xi + 1) + \frac{1}{2}c^2(\xi - 1)^2 + \frac{1}{2}cd} \quad (26)$$

In the simple uniaxial case where  $\kappa_1 = 0$  ( $b = 0$ ) the equations simplify to

$$\hbar\omega_{\alpha,\beta} = \frac{1}{2} \left[ \pm c(\xi - 1) + \sqrt{c^2(1 - \xi)^2 + 4a^2 + 4ac(1 + \xi)} \right] \quad (27)$$

or stated in the anisotropy and exchange field terminology

$$\hbar\omega_{\alpha,\beta} = g\mu_B \left[ \pm \frac{B_E}{2}(\xi - 1) + \sqrt{2B_E B_{A2} + B_E B_{A2}(\xi - 1) + \left( \frac{B_E}{2}(\xi - 1) \right)^2 + B_{A2}^2} \right] \quad (28)$$

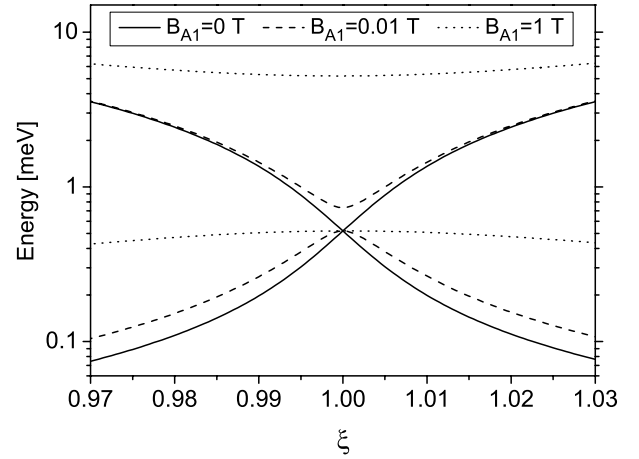
This result is identical to classical calculations for a ferromagnet assuming uniaxial anisotropy [30,31]. However, the calculation has now been performed from a microscopic viewpoint, and can thus be generalized to e.g. include canted spins. The influence of the combined planar and axial anisotropy was not calculated earlier.

### 3 Relation to experimental results

In this section the strong  $\xi$ -dependency of the two resonance energies  $\hbar\omega_\alpha$  and  $\hbar\omega_\beta$  is described and related to experimental data.

Aside from the explicit  $\xi$ -dependency in (28), the exchange field  $B_E$  also depends on  $\xi$  through the exchange interaction  $\mathcal{J}(0)_B^{\text{av}}$ . By definition (13),  $\mathcal{J}(0)_B^{\text{av}}$  depends on  $K$  and  $N_B$ , which are both related to  $\xi$  through the shape and size of the particle.

Figure 1 shows the resonance energies in the situation where the ratio between the number of spins in the two sublattices is close to unity. In this region we can assume that  $B_E$  is independent of  $\xi$ . The exchange field is often very large and in the calculations set to a typical value of  $B_E = 1000$  T. The planar anisotropy field is set to  $B_{A2} = 0.01$  T, which is a realistic order of magnitude for nanoparticles [14,17,18,32]. Three different values of the axial anisotropy are considered, the uniaxial case where  $B_{A1} = 0$  T, the case where the anisotropy contributions are equal in size  $B_{A1} = 0.01$  T and the strongly planar anisotropy case where  $B_{A1} = 1$  T. In the strongly planar case ( $B_{A1} \gg B_{A2}$ ) both precession mode energies  $\hbar\omega$  depend only weakly on the uncompensated moment. As the value of  $B_{A1}$  is reduced, the dependence of  $\hbar\omega_\alpha$  on  $\xi$  becomes stronger. When the two anisotropy terms become equal  $B_{A1} = B_{A2} = 0.01$  T even an uncompensated moment as small as 1% results in a reduction of the energy by a factor of two. In the uniaxial case  $B_{A1} = 0$  this reduction is almost a factor of three.



**Fig. 1.** Energies of the  $\mathbf{q} = 0$  spin wave modes for small values of the uncompensated moment, i.e.  $\xi \simeq 1$ . The upper mode is  $\hbar\omega_\beta$  while the lower mode is  $\hbar\omega_\alpha$ . The energies were calculated with  $B_{A2} = 0.01$  T and  $B_E = 1000$  T. The energies are plotted for  $B_{A1} = 0$ ,  $B_{A1} = B_{A2}$  and  $B_{A1} = 100 B_{A2}$ .

### 3.1 Experimental studies of antiferromagnetic nanoparticles

The magnitude of the uncompensated magnetic moment of antiferromagnetic nanoparticles has in some cases been found to be roughly proportional to  $N^{1/3}$ , where  $N$  is the number of spins in a particle [24,25], corresponding to a situation where the uncompensated moment is due to a more or less random occupation of surface sites [20,24]. Thus,  $|\xi - 1|$  increases rapidly with decreasing particle size.

Inelastic neutron scattering studies of 16 nm  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> particles yielded the excitation energy  $\hbar\omega_\alpha = 0.26$  meV at low temperatures [14]. Previous magnetisation measurements of this sample revealed a value of  $\xi \geq 0.999$  [33]. For these particles,  $B_{A1} \approx 10 B_{A2}$  [15], and thus the energy shift due to the uncompensated moment is according to (25) less than 1%, i.e. negligible.

Also, as reported in reference [18], an inelastic neutron scattering study of plate-shaped NiO nanoparticles suggests anisotropy energies that resemble the planar case with  $B_{A1} \gg B_{A2}$ . In these particles, a value of  $\xi = 0.994$  has been estimated from high-field Mössbauer spectroscopy [25]. It can be seen in Figure 1, that in this case the influence of the uncompensated moment on the excitation energy is again small.

Mössbauer spectroscopy has a time scale of the order of a few nanoseconds, which is longer than the characteristic times of the uniform excitations ( $\sim 10$  ps). Therefore, this technique does not allow measurement of the individual precession states, but only an average over the fluctuations. The uniform excitations give rise to a reduction of the magnetic hyperfine splitting that is inversely proportional to the product of the magnetic anisotropy constant and the volume [8,9], but it does not depend on the spin wave excitation energy [10]. Mössbauer spectroscopy studies have shown that the magnetic anisotropy of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles increases with decreasing particle size [34].



Similar results have been found in studies of nanoparticles of  $\alpha$ -Fe [35] and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> [36]. This can be explained by the increasing influence of surface anisotropy with decreasing particle size. According to equation (22), this should lead to an increase of the spin wave energy. However, such an increase was not observed in a recent inelastic neutron study of 8 nm  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> particles. Indeed, an excitation energy comparable to that found in the 16 nm particles discussed above was observed [17]. The absence of an increase in the excitation energy may, at least qualitatively, be explained by the presence of an uncompensated moment. An  $N^{1/3}$  dependence of the uncompensated moment would suggest that  $\xi \approx 0.99$ . Also,  $B_{A1}$  and  $B_{A2}$  are expected to be of the same order of magnitude in the 8 nm  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> particles [17], resulting in an expected 50% reduction of the excitation energy according to Figure 1. Thus the similarity of the data for 8 nm and 16 nm particles can be explained by the opposite effects of increasing anisotropy and increasing uncompensated moment on the excitation energy.

## 4 Conclusion

The spin wave energy of  $\mathbf{q} = 0$  spin waves (uniform precession) in antiferromagnetic nanoparticles has been calculated from a microscopic Hamiltonian using a coherent potential approximation. Systems of recent experimental interest, with uncompensated moments, planar and axial anisotropy, are considered. In the coherent potential approximation, nanoparticles with uncompensated spins can be considered ferrimagnets, with respect to the  $q = 0$  mode.

Different configurations of such anisotropy ranging from uniaxial to planar anisotropy are presented. It is found that the resonance energy depends strongly on the amount of uncompensated moment in the case of uniaxial anisotropy, with a weaker dependence in the case of strong planar anisotropy.

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