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# Non-uniform magnetodistortive ordering in Jahn–Teller antiferromagnets

V D Ashkinazy and B G Vekhter

Institute of Chemistry, Academy of Sciences of Moldova SSR, Grosul Street 3, 277028  
Kishinev 28, USSR

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**Abstract.** It is shown that the non-uniform phase can exist in Jahn–Teller antiferromagnets under a magnetic field near the boundary of the antiferromagnetic and pseudospin-flop phases. The existence of non-uniform phase results in characteristic peculiarities in the field dependence of the magnetic moment and orthorhombic deformation.

## 1. Introduction

In crystals with a sublattice of Jahn–Teller ions the phonon exchange gives rise to correlations between electronic states of different ions. With a decrease in temperature these correlations cause a transition to the orbitally ordered phase; the corresponding local Jahn–Teller deformations appear to be ordered too—the so-called cooperative Jahn–Teller effect [1]. At the same time the magnetic intersite interaction also exists and can lead to a transition into the magneto-ordered phase. In Jahn–Teller crystals these two possible types of ordering, magnetic and structural, often appear to be in competition. Then only one of them is realized, the one corresponding to the stronger interaction and causing a larger splitting of the degenerate ground states of the Jahn–Teller ions. However, if the favourable ordering appears to be of antiferromagnetic (AFM) type, it can be destabilized by external fields. As a consequence in Jahn–Teller antiferromagnets under a magnetic field the pseudospin-flop (PSF) phase is realized where strong magnetic ordering and weak structural ordering coexist [2, 3]. Near the boundary of the AFM and PSF phases the free energies of both phases are almost equal because the transition between them is of the first order. This means that even weak additional interactions have to be taken into account in such a situation, because they can lead to the appearance of a new phase. As has been shown in [4] such a phase, which is intermediate between the AFM and PSF phases, does appear if weak intrasublattice interactions of a certain kind are accounted for. In the present paper, gradient interactions are considered and the problem of the appearance of a non-uniform phase near the boundary of the AFM and PSF phases is investigated (the appearance of non-uniform ordering in antiferromagnets under a magnetic field may serve as an analogue of such a situation [5]).

## 2. AFM tetragonal crystal with non-Kramers doublet

As in [2-4] we consider the case of an AFM tetragonal crystal with a non-Kramers doublet as a ground state of one of the ion sublattices. Crystals such as  $\text{HoPO}_4$  and  $\text{HoAsO}_4$  may serve as examples [1]. It is convenient to describe the non-Kramers doublet by a pseudospin  $S = \frac{1}{2}$ . One can choose the basis with the  $S_z$ -component corresponding to the magnetic dipole moment along the tetragonal  $c$  axis and the  $S_x$  and  $S_y$  components corresponding to electron quadrupole moments in the basic plane. The Hamiltonian which accounts for both the magnetic and the Jahn-Teller (of  $b_{1g}$  type only; see [2]) quadrupole-quadrupole interactions is as follows:

$$\mathcal{H} = - \sum_{mn} (J_{mn} S_z^m S_z^n + A_{mn} S_x^m S_x^n) - \frac{1}{2} g\beta H \sum_m S_z^m. \quad (1)$$

To analyse the non-uniform distribution of  $S^n$  let us proceed as is usually done, from the Hamiltonian (1) to its phenomenological analogue, i.e. energy functional  $E$ :

$$E = \int w \, dV = \int (w_0 + w') \, dV \quad (2)$$

separating the uniform term  $w_0$  and non-uniform term  $w'$ . The uniform term may be written in the form

$$w_0 = -J S_z^I(\mathbf{r}) S_z^{II}(\mathbf{r}) - A S_x^I(\mathbf{r}) S_x^{II}(\mathbf{r}) - h [S_z^I(\mathbf{r}) + S_z^{II}(\mathbf{r})]. \quad (3)$$

Here the value of mean magnetic field  $J = \sum_m J_{mn} / \Omega_0$  is negative for antiferromagnets;  $A = \sum_m A_{mn} / \Omega_0$  is the value of the mean quadrupole field, which is proposed to be positive, as in the majority of rare-earth tetragonal Jahn-Teller crystals [1];  $h = \frac{1}{2} g\beta H / \Omega_0$ , where  $\Omega_0$  is the elementary cell volume. Only intersublattice interactions are taken into account. The magnetic and quadrupole moments of elementary volume are proportional to  $m_z(\mathbf{r}) = \frac{1}{2} [S_z^I(\mathbf{r}) + S_z^{II}(\mathbf{r})]$  and  $m_x(\mathbf{r}) = \frac{1}{2} [S_x^I(\mathbf{r}) + S_x^{II}(\mathbf{r})]$ , respectively. Note that the existence of a non-zero quadrupole moment  $m_x(\mathbf{r})$  in the basic plane causes the simultaneous appearance of a corresponding orthorhombic distortion that is proportional to  $m_x(x)$  [2]. It is convenient to introduce also the AFM and antiferrodistortive parameters  $l_z(\mathbf{r}) = \frac{1}{2} [S_z^I(\mathbf{r}) - S_z^{II}(\mathbf{r})]$  and  $l_x(\mathbf{r}) = \frac{1}{2} [S_x^I(\mathbf{r}) - S_x^{II}(\mathbf{r})]$ ; the relations between  $S_{x,z}^i$ ,  $m_{x,z}$  and  $l_{x,z}$  are  $S_x^{I,II} = m_x \pm l_x$  and  $S_z^{I,II} = m_z \pm l_z$ .

The non-uniform term  $w'$  may be written as a series over space derivatives of the  $S_{x,z}^{I,II}(\mathbf{r})$  order parameters; it is more convenient to use derivatives of  $m_{x,z}(\mathbf{r})$  and  $l_{x,z}(\mathbf{r})$ . As the appearance of an invariant linear term in the first derivatives is forbidden in centrosymmetric tetragonal crystals the first non-vanishing terms in  $w'$  are

$$w'_1 = \sum_{\alpha\beta} \left[ \left( \frac{\partial m_\alpha}{\partial x_\beta} \right)^2 \gamma_{\alpha\beta}^m + \left( \frac{\partial l_\alpha}{\partial x_\beta} \right)^2 \gamma_{\alpha\beta}^l \right] \quad (4)$$

where  $\alpha = x, z$  and  $x_{1,2,3} = x, y, z$ . The only terms in (4) that can give rise to non-uniform orderings are those with negative  $\gamma$ . It is known that non-uniform structures often result from competition between interactions with nearest and next-nearest neighbours (see, e.g. [6]). In the Jahn-Teller crystals under consideration the vibronic

coupling leads to quadrupole-quadrupole interactions of a ferrotype and of a long range [1]. This means that there is no competition between quadrupole interactions with different coordinating spheres and consequently the coefficients of the space derivatives of  $m_x$  and  $l_x$  has to be positive. The magnetic interactions of short-range nature with different coordinating spheres, in contrast, often have different signs; this may result in the well known non-uniform structures in magnetics [6]. In compounds with a stable AFM structure, as in the case under consideration, the coefficient of the space derivatives of the AFM parameters  $l_z$  obviously has to be positive. At the same time the instability of ferromagnetic ordering means that the coefficient  $\gamma$  corresponding to the FM parameter  $m_z$  has to be negative. It is obvious that non-uniform ordering does arise when the decrease in energy caused by terms with derivatives of  $m_x$  is larger than the increase in energy caused by other terms from (4) with positive  $\gamma$ . Below we suppose that this condition is fulfilled, i.e. the coefficients of the derivatives of  $m_x$  are much greater in value than the other coefficients in (4). Then (4) can be rewritten as follows:

$$w'_1 = \gamma_{\parallel} (\partial m_x / \partial z)^2 + \gamma_{\perp} \left[ (\partial m_x / \partial x)^2 + (\partial m_x / \partial y)^2 \right]. \quad (5)$$

If the coefficients  $\gamma_{\parallel}$  and  $\gamma_{\perp}$  in (5) are negative, the more frequently oscillating is the non-uniform structure, then the greater is the energy gain. To stabilize the evolution of the non-uniform phase the invariants containing higher derivatives of  $S_{x,z}^i(\mathbf{r})$  with positive coefficients must be taken into account. Because of these invariants the free energy of the non-uniform phase increases and  $S_{x,z}^i$  have to change gradually as a result. Accounting for the second derivatives of  $m_x$ , we receive for  $w'$  finally

$$w' = \gamma_{\parallel} (\partial m_x / \partial z)^2 + \gamma_{\perp} \left[ (\partial m_x / \partial x)^2 + (\partial m_x / \partial y)^2 \right] + \alpha_{\parallel} (\partial^2 m_x / \partial z^2)^2 + \alpha_{\perp} \left[ (\partial^2 m_x / \partial x^2)^2 + (\partial^2 m_x / \partial y^2)^2 \right]. \quad (6)$$

### 3. Non-uniform structures at low temperatures

The general analysis of possible non-uniform structures is known to be rather complicated. So we restrict ourselves to the case of low temperatures ( $T \ll |J|, |A|$ ); in this case the relation  $(\bar{S}_x^n)^2 + (\bar{S}_z^n)^2 = 1$  is fulfilled:

$$S_x^{\alpha}(\mathbf{r})^2 + S_z^{\alpha}(\mathbf{r})^2 = 1 \quad \alpha = \text{I, II} \quad (7)$$

in the continuum model. Condition (7) confines the number of independent order parameters to two only instead of the initial four  $S_{x,z}^{\text{I,II}}$ . The two parameters can conveniently be chosen as  $m$  and  $\theta$ , where  $m = \sqrt{m_x^2 + m_z^2}$ ,  $\tan \theta = m_x / m_z$ . One can easily find that

$$\begin{aligned} m_z &= m \cos \theta & l_x &= \sqrt{1 - m^2} \sin \theta \\ m_x &= m \sin \theta & l_z &= \sqrt{1 - m^2} \cos \theta. \end{aligned} \quad (8)$$

In the variables  $m$  and  $\theta$  the uniform part  $w_0$  is

$$w_0 = -J(m^2 - \sin^2 \theta) - A(m^2 - \cos^2 \theta) - 2hm \cos \theta \quad (9)$$

whereas, in the non-uniform part (6),  $m \cos \theta$  has to be substituted instead of  $m_z$ .

Let us consider first pure uniform structures. Minimizing  $w_0$  over  $\theta$ , one finds that

$$\cos \theta = \begin{cases} hm/h_2 & h \leq h_2 \\ 0 & h > h_2 \end{cases} \quad (10)$$

and inserting (10) into (9) gives

$$w_0 = \begin{cases} J + [(h_1^2 - h^2)/h_2]m^2 & h \leq h_2 \\ -J - 2h & h > h_2 \end{cases} \quad (11)$$

$$h_1 = \sqrt{(-J - A)(-J + A)} \quad h_2 = -J + A. \quad (12)$$

From equation (11) it follows immediately that at  $h < h_1$  the coefficient for  $m^2$  is positive; thus the phase with  $m = 0$  is the most stable. In accordance with (10) and (8) the condition  $m = 0$  means that  $S_z^I = -S_z^{II} = 1$  and  $S_x^i = 0$ , i.e. this solution corresponds to AFM phase without quadrupole and structural orderings. At  $h > h_1$  the coefficient for  $m^2$  in (10) becomes negative and the most stable phase appears to be that with  $m = 1$ . In accordance with (10) and (8) it corresponds to the magnetodistortive PSF phase where both magnetic ordering and quadrupole ordering exist:

$$S_z^{I,II} = h/h_2 \quad S_x^i = S_x^{II} = \pm \sqrt{1 - (h/h_2)^2}. \quad (13)$$

Two signs of  $S_x^{I,II}$  correspond to the two possible orientations of the Jahn-Teller orthorhombic deformation. Finally at  $h > h_2$  the crystal is in the paramagnetic (PM) phase with  $S_z^I = S_z^{II} = 1$ ,  $S_x^i = 0$ . The energies of these phases are

$$E_{AF} = JV \quad E_{PSF} = V[J + (h_1^2 - h^2)/h_2] \quad E_{PM} = V(-J - 2h). \quad (14)$$

$V$  is the crystal volume. This is just the result obtained in [2, 3].

Let us now take account of the non-uniform contribution. From equations (6) and (10) one obtains

$$\begin{aligned} w' = & -\gamma_{\parallel}(h^2/h_2^2)4m^2(\partial m/\partial z)^2 - \gamma_{\perp}(h^2/h_2^2)4m^2[(\partial m/\partial x)^2 + (\partial m/\partial y)^2] \\ & + 4\alpha_{\parallel}(h^2/h_2^2)[m \partial^2 m/\partial z^2 + (\partial m/\partial z)^2]^2 + 4\alpha_{\perp}(h^2/h_2^2)\{[m \partial^2 m/\partial x^2 \\ & + (\partial m/\partial x)^2]^2 + [m \partial^2 m/\partial y^2 + (\partial m/\partial y)^2]^2\}. \end{aligned} \quad (15)$$

The behaviour of  $m(\mathbf{r})$  is determined from the condition of the functional  $E$  minima. However, in the general case, such a minimization procedure cannot be done exactly. That is why another way is used as a rule, i.e. one chooses a certain non-uniform distribution  $m(\mathbf{r})$  and compares its energy with the energy of uniform structures. Consider first the distribution depending on  $z$  only, i.e. the one-dimensional non-uniform structure. This is the case with  $\gamma_{\parallel} < 0$ ,  $\gamma_{\perp} > 0$ , when  $S_{x,z}^i(\mathbf{r})$  do not depend upon  $x$  and  $y$ . So we choose

$$m = \sin^2(kz). \quad (16)$$

In accordance with (16), while moving along the  $z$  axis, one goes from a pure AFM region (at  $z = 0$ , where  $m = 0$ ) to a PSF region (at  $z = \pi/2k$ , where  $m = 1$ ). In the intermediate range between  $z = 0$  and  $z = \pi/2k$ ,  $S_z^I$  decreases from  $S_z^I = 1$  to  $S_z^I = h/h_2$  and  $S_z^{II}$  increases from  $S_z^{II} = -1$  to  $S_z^{II} = h/h_2$ . As for  $S_x^{I,II}$  describing the sublattice quadrupole moments, they are equal to zero at  $z = 0$ ; then their absolute values increase with increase in  $z$  ( $S_x^I$  monotonically and  $S_x^{II}$  non-monotonically) and reach the values  $S_x^I = S_x^{II} = \sqrt{1 - (h/h_2)^2}$  at  $z = \pi/2k$ .

The non-uniform distribution (16) possesses in accordance with (15) the following energy:

$$E_{NU} = V[J + \frac{3}{8}(h_1^2 - h^2)/h_2 + \frac{5}{8}\gamma_{||}(h^2/h_2^2)k^2 + 4\alpha_{||}(h^2/h_2^2)k^4]. \tag{17}$$

The energy  $E_{NU}$  has its minimal value at  $k = k_0$ :

$$E_{NU}(k_0) = V[J + \frac{3}{8}(h_1^2 - h^2)/h_2 - \chi(h^2/h_2^2)(\gamma_{||}^2/\alpha_{||})] \quad k_0 = \frac{1}{8}\sqrt{5\gamma_{||}/\alpha_{||}} \tag{18}$$

where  $\chi = 0.024$ . Comparing this value with (14) one finds that there always is the field range  $h_{NU}^1 < h < h_{NU}^2$  where the non-uniform structure is more stable than the AFM and PSF structures (at any values of  $\gamma$  and  $\alpha$ ):

$$\begin{aligned} h_{NU}^1 &= h_1(1 + \gamma^2\chi_1/\alpha h_2)^{-1/2} \\ h_{NU}^2 &= h_1(1 - \gamma^2\chi_2/\alpha h_2)^{-1/2} \quad \chi_1 = 0.065 \quad \chi_2 = 0.039. \end{aligned} \tag{19}$$

The AFM and PSF phases are realized at  $h < h_{NU}^1$  and  $h > h_{NU}^2$  respectively. Transitions from a non-uniform structure to the AFM and PSF phases are of the first order.

Figure 1 shows the field dependence of the magnetic moment parameter  $M_z = (1/V) \int m_z dV$ . One can see that the one-step increase in  $M_z$  that took place at uniform AFM ordering and PSF ordering [3] is now divided into two steps at  $h_{NU}^1$  and  $h_{NU}^2$ , inside this field interval  $M_z(h) = \frac{3}{8}h/h_2$  which is proportional to the field. Figure 2 shows the field dependence of  $Q_x = (1/V) \int m_x dV$ , the parameter of crystal orthorhombic deformation.

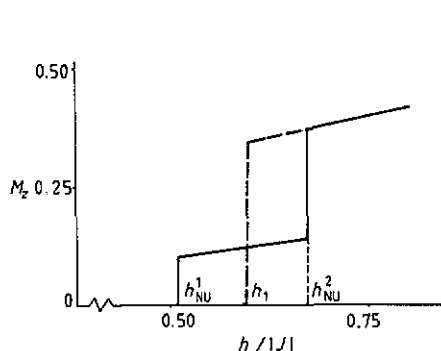


Figure 1. Field dependence of the non-uniform phase magnetic parameter  $M_z$  ( $A/|J| = 0.8$ ;  $\gamma_{||}^2/\alpha_{||}|J| = 10$ ): - - -,  $M_z(H)$  behaviour when the non-uniform phase is absent.

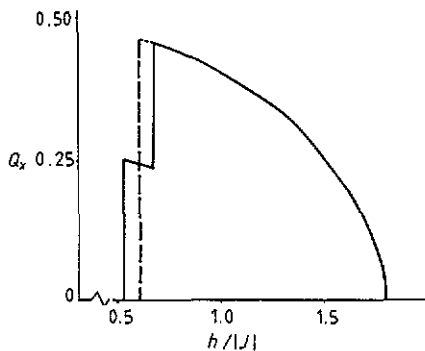


Figure 2. Behaviour of the non-uniform phase deformation parameter  $Q_x$  ( $A/|J| = 0.8$ ;  $\gamma_{||}^2/\alpha_{||}|J| = 10$ ): - - -,  $Q_x(H)$  behaviour when the non-uniform phase is absent.

Let us now consider the  $(x, y)$ -dependent ordering at  $\gamma_{\parallel} > 0$ ,  $\gamma_{\perp} < 0$ . In this case, non-uniform structures can be realized that are more complicated than those of the one-dimensional case discussed above. To illustrate this we examine below the non-uniform structure of vortex type (for pure magnetic materials, vortex type structures were examined in [7]). We suppose that  $m(\mathbf{r}) = m(\rho/\rho_0)$ , where  $\rho = \sqrt{x^2 + y^2}$  is the distance from the vortex axis that is parallel to the crystal  $c$  axis to the  $\mathbf{r}$  point; the vortex radius  $\rho_0$  is the distance from the vortex axis to the points where the non-uniform distribution converts into the uniform distribution. Then for the vortex energy one can obtain the following expressions:

$$\epsilon_v = \pi\rho_0^2 l [J + D(h_1^2 - h^2)/h_2 - \gamma_{\perp}(h^2/h_2^2)(B/\rho_0^2) + \alpha_{\perp}(h^2/h_2^2)(C/\rho_0^4)] \quad (20)$$

$$D = 2 \int_0^1 m^2(x) x dx \quad B = 2 \int_0^1 \left( \frac{\partial m}{\partial x} \right)^2 x dx$$

$$C = 2 \int_0^1 \left[ \left( \frac{\partial^2 m}{\partial x^2} \right)^2 + \frac{3}{4} \frac{(\partial m / \partial x)^2}{x^2} \right] x dx \quad x = \frac{\rho}{\rho_0} \quad (21)$$

The number of vortices appearing in the unit volume is  $N = p\pi^{-1}\rho_0^{-2}l^{-1}$ , where  $l$  is the vortex length and the coefficient  $p$  is determined by the method of vortex packing ( $p = \pi(2\sqrt{3})^{-1}$  for triangular lattice,  $p = \pi/4$  for a square lattice, etc). Then the energy of unit volume of the non-uniform vortex phase  $E_v = N\epsilon_v$  takes the form

$$E_v = p[J + D(h_1^2 - h^2)/h_2 - \gamma_{\perp}(h^2/h_2^2)(B/\rho_0^2) + \alpha_{\perp}(h^2/h_2^2)(C/\rho_0^4)]. \quad (22)$$

The energy  $E_v$  has its minimum value at  $\rho_0 = \rho_{\min}$ :

$$\rho_{\min} = \sqrt{(2\alpha_{\perp}/\gamma_{\perp})(C/B)} \quad (23)$$

$$E_v(\rho_{\min}) = p[J + D(h_1^2 - h^2)/h_2 - (\gamma_{\perp}^2/4\alpha_{\perp})(h^2/h_2^2)(B^2/C)].$$

On the other hand, if the volume occupied by vortices were in the uniform, AFM or PSF phases, its energy density would be

$$E_{AF} = JN\pi\rho_0^2 l = Jp \quad E_{PSF} = p[J + (h_1^2 - h^2)/h_2]. \quad (24)$$

Comparing these energies (23) and (24), we come to the following conclusions: at  $h = h_{v1}$  the crystal jumps from the AFM phase to the vortex phase and then at  $h = h_{v2}$  another first-order transition takes place from the vortex phase to the PSF phase:

$$h_{v1} = h_1(1 + \gamma_{\perp}^2 B^2 / 4\alpha_{\perp} h_2 DC)^{-1/2} \quad (25)$$

$$h_{v2} = h_1[1 - \gamma_{\perp}^2 B^2 / 4\alpha_{\perp} h_2(1 - D)C]^{-1/2}.$$

The values of  $h_{v1}$  and  $h_{v2}$  are determined by the parameters  $B$ ,  $C$  and  $D$  that depend upon  $m(\mathbf{r})$  in accordance with (21).

Up to now we have not made any assumptions about the concrete behaviour of  $m(\rho)$ , which determines the distribution of the magnetic moment and the orthorhombic deformation inside the vortex. There may be two qualitatively different types of  $m(\mathbf{r})$  behaviour:

- (i) vortex I with  $m(0) = 1$  and  $m(\rho_0) = 0$ ;
- (ii) vortex II with  $m(0) = 0$ ,  $m(\rho_0) = 1$ .

It is the PSF phase that is realized on the axis of vortex I, and it is the AFM phase at its boundary. While moving from vortex boundary to its centre the magnetic moment and absolute value of the quadrupole moment increase from zero to  $h/h_2$  and  $\sqrt{1 - (h/h_2)^2}$ , respectively. There is quite the opposite picture for vortex II, i.e. the AFM phase on the axis and the PSF phase at the boundary. These two distributions may be described by the following relations:

$$m^I = \begin{cases} \cos^2(\pi\rho/2\rho_0) & \rho \leq \rho_0 \\ 0 & \rho > \rho_0 \end{cases} \tag{26}$$

$$m^{II} = \begin{cases} \sin^2(\pi\rho/2\rho_0) & \rho \leq \rho_0 \\ 1 & \rho > \rho_0 \end{cases}$$

Using (26), one finds from (21) that

$$D_I = 0.28 \quad D_{II} = 0.72 \quad B_I = B_{II} = 1.24 \quad C_I = C_{II} = 21.0. \tag{27}$$

Figure 3 shows the field dependence of the energies of the AFM, PSF and non-uniform phases, calculated in accordance with (23) and (24). Comparing these energies, one concludes that first at  $h = h_{v1}$  vortices I appear and then at  $h = h_1$  ( $h_1$  is given by equation (12)) they are changed by vortices II; the latter disappear at  $h \geq h_{v2}$ . It is conceivable that in passing from vortices I to vortices II the uniform areas between vortices I (they are in AFM phase) become the centres of vortices II.

The field dependence of the magnetic moment of the vortex structure is shown in figure 4. There are three jumps of  $M_z$ , at  $h = h_{v1}, h_1, h_{v2}$ . At  $h_{v1} < h < h_{v2}$  the magnetic moments of vortex lattices are given by the expressions

$$M_z = pD_I h/h_2 \quad \text{vortices I} \tag{28}$$

$$M_z = pD_{II} h/h_2 \quad \text{vortices II.}$$

That is, in vortex phases the magnetic moment is linear in field, as it is for the non-uniform structure of the distribution depending on  $z$  only.

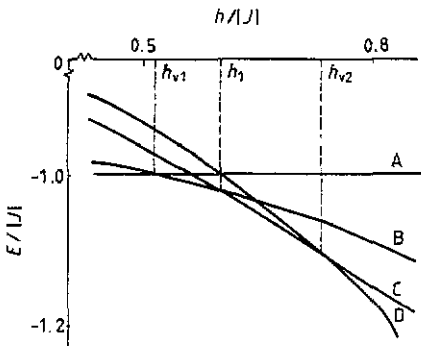


Figure 3. Field dependence of energies of AFM (curve A), vortex I (curve B), vortex II (curve C) and PSF (curve D) phases ( $A/|J| = 0.8$ ;  $\gamma_1^2/\alpha_\perp|J| = 10$ ).

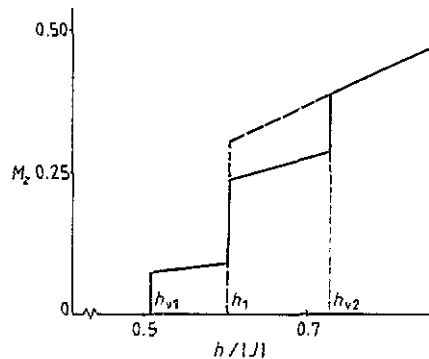


Figure 4. Field dependence of the vortex magnetic parameter  $M_z$  ( $A/|J| = 0.8$ ;  $\gamma_1^2/\alpha_\perp|J| = 10$ ): - - -,  $M_z(H)$  behaviour when the non-uniform phase is absent.



In the above equations (13), there are two possible signs of the orthorhombic deformation in the PSF phase; the situation with the crystal quadrupole moment and corresponding crystal orthorhombic deformation for a vortex structure is more complicated. For the vortex I structure the quadrupole moment and orthorhombic deformation vanish at the boundary of the vortices; this means that the quadrupole moments (deformations) of different vortices I are not correlated. Therefore no definite conclusion about the quadrupole moment of the whole crystal can be drawn in such a situation; however, because of the random distribution of deformation signs the total quadrupole moment (deformation) evidently has to be close to zero. With vortices II, the uniform areas between the vortices are in the PSF phase, and deformation in these areas is different from zero. As a consequence the deformations inside the different vortices II have to have the same sign; otherwise the order parameters possess discontinuity at the boundary of the uniform and non-uniform areas. The corresponding field dependence of  $Q_x$  resembles that in figure 2; the first jump of  $Q_x$  takes place at  $h = h_1$ , when vortices I are changed into vortices II.

#### 4. Conclusion

In conclusion we wish to emphasize once more that the investigation of Jahn-Teller AFM behaviour under a magnetic field  $H$  can give important information about the weak interactions, which are not manifested directly at  $H = 0$ . The gradient interactions discussed above which initiate the non-uniform ordering are shown to cause the pronounced peculiarities in the field dependence of the magnetic moment and Jahn-Teller deformation. The investigation of these features allows one to appreciate the values of the corresponding microscopic parameters and to clarify the picture of different types of ordering.

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