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The magnetic field behaviour of a Haldane-gap antiferromagnet

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Abstract. We investigate the magnetic field behaviour of an antiferromagnetic Heisenberg spin-1 chain with the most general single-ion anisotropy. We discuss the regime in which the magnetic field is below the transition value. The splitting of the Haldane triplet is obtained as a function of a field applied in an arbitrary orientation by means of a Lanczös exact diagonalization of chains of up to 16 spins. Our results are well summarized in terms of a first-order perturbation theory. We explain various level crossings that occur by the existence of discrete symmetries. A discussion is given of the electron-spin-resonance and neutron-scattering experiments on the compound $Ni(C_2H_8N_2)_2NO_2ClO_4$ (NENP).

1. Introduction

There is good evidence that the integer-spin Heisenberg antiferromagnetic chains have a gap, as suggested by Haldane [1]. This is established on the theoretical side by various techniques including finite-size calculations as well as field theoretic arguments [2]. On the experimental side the first evidence [3] came from $CsNiCl_3$: neutron scattering (NS) revealed an excitation gap. Since this compound is only moderately one dimensional, parasitic three-dimensional effects complicate the picture. On the other hand, the compound [4] $Ni(C_2H_8N_2)_2NO_2ClO_4$, abbreviated as NENP, is much more one dimensional and remains in a magnetically disordered state even at very low temperature. Zero-field NS experiments [5] have clearly shown the existence of the Haldane triplet split by easy-plane anisotropy. In addition, a number of other measurements have been performed [5–8] in a magnetic field: susceptibility, high-field magnetization, and NS in a finite field. The application of a magnetic field leads to a Zeeman splitting of the Haldane triplet and one member of this triplet crosses the ground state at a critical value H_c that depends on the field orientation. This is clearly seen in NS experiments where all members of the triplet can be followed individually [9]. Experiments using the electron-spin-resonance (ESR) technique are in excellent agreement [10] with NS as is the case for far-infrared spectroscopy measurements [11] and there is at the present time a satisfactory picture of the behaviour of NENP from the experimental point of view.

On the theoretical side, effective-quantum-field theories have been used to predict the magnetic-field behaviour of the spin-1 chain Heisenberg Hamiltonian that models the magnetic properties of NENP. In fact the original work of Haldane showed that, in the large-integer-spin limit, the antiferromagnetic spin chain is described in the low-energy limit by

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an O(3) non-linear sigma model. This non-trivial field theory is difficult to study and, based on the large-N limit of the O(N) model, it has been suggested that a simple theory with three massive bosonic fields might be an appropriate effective theory of the spin-1 chain. It is then possible to obtain the behaviour [12, 13] of the system in a magnetic field.

Another possibility has been suggested starting from an integrable chain [14]. It is known that the spin-1 Hamiltonian $\mathcal{H}_0 = \sum_i S_i \cdot S_{i+1} - (S_i \cdot S_{i+1})^2$ is solvable by the Bethe *ansatz* technique [15] and leads to a massless theory. This massless theory is characterized by an $SU(2)_{k=2}$ symmetry and can be realized by three (massless) Majorana fermions. As one perturbs the Hamiltonian $\mathcal{H}_0$ towards the pure Heisenberg Hamiltonian without biquadratic coupling, it is natural in the framework of the Haldane conjecture to expect that these fermions become massive. One can then use a theory of three free massive Majorana fermions to approximate the Heisenberg chain. These two theoretical approaches are not in complete agreement and it is thus interesting to have results of a completely different nature, based on numerical studies of finite-chain diagonalization.

In this paper, we present the results of our study of the field behaviour of a spin-1 chain including realistic single-ion anisotropies of the most general kind. We diagonalize by means of a Lanczös algorithm chains of up to 16 spins under a magnetic field applied in various positions. Our findings are neatly summarized by a simple perturbation calculation that may be used as a practical tool to obtain the field behaviour of a Haldane magnet. When the applied field becomes strong enough there is a phase transition towards a magnetically ordered phase [12, 13]. In this paper we will restrict ourselves to the singlet phase where the Haldane gap is not destroyed. We give a discussion of the various level crossings that may or may not appear depending on the field orientation with respect to the symmetry axis of the crystal. Section 2 contains the treatment of the magnetic field as a perturbation. Section 3 explains the Lanczös results as well as their relationships with the perturbative expansion. Section 4 contains our conclusions and a discussion of NENP experiments. An appendix contains explicit formulas for the gaps from the perturbative treatment of the magnetic field.

2. The perturbative results

We focus on the microscopic Hamiltonian of a spin-1 antiferromagnetic chain in an applied field and single-ion anisotropy:

$$\mathcal{H} = J \sum_i S_i \cdot S_{i+1} + D(S_i^z)^2 + E[(S_i^x)^2 - (S_i^y)^2] - \boldsymbol{H} \cdot S_i. \tag{2.1}$$

Here S_i are quantum spins $S = 1$ and we include the Bohr magneton and the Landé g factors in the definition of the magnetic field. The exchange coupling J is taken to be positive, i.e. antiferromagnetic. Below we set $J = 1$. The terms D and E in equation (2.1) parametrize the most general single-ion anisotropy. We work with periodic boundary conditions. In zero field and in the absence of anisotropy ($D = E = 0$) the Hamiltonian (2.1) is invariant under the full SU(2) rotation group. If the D term is non-zero then the symmetry is broken to a residual U(1) subgroup of rotations around the Z axis. If, in addition to D, there is some further in-plane anisotropy (non-zero E) even this U(1) is broken. However in this case there are still discrete remnants of the initial SU(2): the system is invariant under π rotations around the coordinate axis X, Y, Z. These symmetry operations are denoted by R_x^π, R_y^π and R_z^π, respectively, in this article.

If we now add a magnetic field, there is further symmetry reduction: when $\boldsymbol{H}$ is in a generic position with respect to the coordinate axis, even the discrete operations R_x^π, R_y^π, R_z^π are lost. However, there are some special orientations of $\boldsymbol{H}$ that retain discrete symmetries: if $\boldsymbol{H}$ lies along the α axis, the symmetry R_α^π is conserved. This corresponds simply to rotation around the magnetic field axis. These extra symmetries [16] explain the various level crossings that are found in our exact diagonalization studies reported in section 3.

We now discuss the application of perturbation theory with respect to the terms D, E and $\boldsymbol{H}$ terms in Hamiltonian (2.1). We write equation (2.1) as

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_1 \\ \mathcal{H}_0 &= \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \\ \mathcal{H}_1 &= \sum_i D(S_i^z)^2 + E[(S_i^x)^2 - (S_i^y)^2] - \boldsymbol{H} \cdot \boldsymbol{S}_i. \end{aligned} \tag{2.2}$$

The Hamiltonian $\mathcal{H}_0$ has full rotational symmetry and its levels can thus be classified according to their spin. We focus on the effect of the perturbation on a singlet and a triplet state. We know that the ground state of $\mathcal{H}_0$ is in fact a singlet with chain momentum $K = 0$ and that the first excited state is a triplet with momentum $K = \pi$. Our statements about the effect of the perturbation are general since they are dictated by the Wigner–Eckart theorem.

Let us first discuss the case of a singlet state $|0\rangle$. Due to complete isotropy, the following equalities hold:

$$\langle 0|\sum_i (S_i^x)^2|0\rangle = \langle 0|\sum_i (S_i^y)^2|0\rangle = \langle 0|\sum_i (S_i^z)^2|0\rangle = \tfrac{1}{3}NS(S+1) = \tfrac{2}{3}N. \tag{2.3}$$

In addition the vector $\langle 0|\sum_i \boldsymbol{S}_i|0\rangle$ is zero. We thus obtain the first-order shift of the singlet energy

$$E^{(1)} = E_0 + D\langle 0|\sum_i (S_i^z)^2|0\rangle = E_0 + \tfrac{2}{3}DN. \tag{2.4}$$

We note that there is no effect from the in-plane E-term or $\boldsymbol{H}$. We now discuss the triplet splitting in zero field. In the standard basis the triplet states are denoted $|1m\rangle$, $m = -1, 0, +1$. Perturbation theory involves matrix elements of the following operator:

$$\mathcal{O}^{\alpha\beta} = \sum_i S_i^\alpha S_i^\beta - \tfrac{2}{3}\delta^{\alpha\beta}N. \tag{2.5}$$

This is a spin-2 irreducible tensor operator since it transforms as a traceless symmetric tensor. Its standard components are denoted $\mathcal{O}^{(2M)}$, $M = -2, \ldots, +2$. The Wigner–Eckart theorem implies that the matrix elements in a triplet state of such an operator are related by

$$\langle 1m|\mathcal{O}^{(2M)}|1m'\rangle = C\langle 1m|21Mm'\rangle. \tag{2.6}$$

In this equation $\langle 1m|21Mm'\rangle$ is the Clebsch–Gordan coefficient coupling two spin-1 states to a spin-2 state. Thus perturbation theory is characterized by a single coefficient C (to first order). This is easily found when working out matrix elements in the canonical basis $|x\rangle, |y\rangle, |z\rangle$ rather than using the standard basis. We consider the matrix elements

$$\langle\alpha|\sum_i (S_i^\beta)^2|\gamma\rangle. \tag{2.7}$$

Application of a π rotation shows that this element is zero if α and γ are distinct. In this case there are only two different matrix elements. We can choose

$$\begin{aligned}&\langle x|\sum_i (S_i^z)^2|x\rangle (\equiv a)\\ &\langle x|\sum_i (S_i^x)^2|x\rangle (\equiv b).\end{aligned} \tag{2.8}$$

In addition one notes that $b + 2a = NS(S+1) = 2N$. The perturbation $\mathcal{H}_S = \sum_i D(S_i^z)^2 + E[(S_i^x)^2 - (S_i^y)^2]$ in the canonical basis for the triplet can thus be written as

$$\mathcal{H}_S = \begin{pmatrix} aD + (2N-3a)E & 0 & 0 \\ 0 & aD + (3a-2N)E & 0 \\ 0 & 0 & 2(N-a)D \end{pmatrix}. \tag{2.9}$$

As dictated by the Wigner–Eckart theorem there is only one coefficient that characterizes the perturbation. Subtracting the ground-state energy one is led to the following gap values:

$$\begin{aligned}\Delta_x &= \Delta - \kappa D + 3\kappa E\\ \Delta_y &= \Delta - \kappa D - 3\kappa E\\ \Delta_z &= \Delta + 2\kappa D.\end{aligned} \tag{2.10}$$

In this equation Δ is the unperturbed triplet–singlet gap and we note that $\kappa = \frac{2}{3}N - a$. The coefficient a is extensive but the difference $\frac{2}{3}N - a$ is finite in the thermodynamic limit since κ appears in gap values. The value of κ is not dictated by rotational symmetry of course and its numerical value depends for example on the moment of the triplet. When $E = 0$ this splitting has been studied in detail [17, 18] for the Haldane triplet with chain momentum π, which is the lowest-lying triplet. We note that already for $D \simeq 0.2J$ there are deviations from the previous perturbation theory: the slopes with D of the two gaps are found to be

$$\begin{aligned}\Delta_x &= \Delta_y = \Delta - 0.57D\\ \Delta_z &= \Delta + 1.41D.\end{aligned} \tag{2.11}$$

This is the best linear fit of the Lanczös results between $D = 0.10J$ and $D = 0.25J$. The slope ratio is already slightly different from two as given by equation (2.10). The curvature of the gaps as functions of D is clearly seen in the data of [18]. In fact a fit including quadratic terms in D of the same data leads to the following result:

$$\begin{aligned}\Delta_x &= \Delta_y = \Delta - 0.668D + 0.269D^2\\ \Delta_z &= \Delta + 1.357D + 0.135D^2.\end{aligned} \tag{2.12}$$

The first-order terms satisfy the perturbative results (2.10) and we clearly see the deviation from first order. For practical purposes it is simpler to use the fits (2.11).

We now add the magnetic field to the perturbative treatment. The ground state, being a singlet, is not affected at first order and only the triplet changes. The matrix of the perturbation in the canonical basis is then

$$\mathcal{H}_S - \boldsymbol{H}\cdot\boldsymbol{S} = \begin{pmatrix} p_x & \mathrm{i}H_z & -\mathrm{i}H_y \\ -\mathrm{i}H_z & p_y & \mathrm{i}H_x \\ \mathrm{i}H_y & -\mathrm{i}H_x & p_z \end{pmatrix}. \tag{2.13}$$

The quantities p_α denote the diagonal matrix elements of equation (2.9). Shifting the origin of the energies it is convenient to set $p_\alpha = \Delta_\alpha$ and then the eigenenergies of (2.13) are directly the gaps. In section 3 we show that the resulting values are always extremely close to the Lanczös results when the magnetic field is below the critical value. Diagonalization of (2.13) does not lead to compact formulas except when the field lies along one of the symmetry axes. If $\boldsymbol{H}$ lies along the direction γ we denote its only non-zero component by H_γ. The eigenvalue Δ_γ is unperturbed and the two other eigenvalues are given by

$$\Delta^{\pm} = \tfrac{1}{2}\{\Delta_\alpha + \Delta_\beta \pm [(\Delta_\alpha - \Delta_\beta)^2 + 4H_\gamma^2]^{1/2}\}. \tag{2.14}$$

Here α and β are the two other coordinates. There is hyperbolic repulsion of the two gaps Δ^+ and Δ^-. The smallest gap Δ^- goes to zero for a critical value $H_c^2 = \Delta_\alpha \Delta_\beta$. At large fields the asymptotic behaviour of the gaps is linear. Of course the crossing of one member of the triplet with the ground state signals a phase transition [12, 13] beyond which we do not expect to gain anything from a simple perturbative calculation since other states with higher spins also cross the ground state above H_c.

For the convenience of the reader we give in the appendix the general formulas for the gaps resulting from diagonalization of the matrix (2.13).

It is interesting to note that this hyperbolic behaviour (2.14) is exactly what is found in the fermionic effective theory [14] for states with $K = \pi$. When the field becomes large and parallel to a coordinate axis the eigenstates of (2.13) take a simple form: they are given by $|\alpha) \pm i|\beta)$. We note that the vanishing of Δ^- at H_c occurs linearly contrary to the free-boson prediction.

If the gap value Δ_γ (which does not move with the field) lies above or below the two gaps Δ_α and Δ_β there is in general a crossing of levels between one of the gaps $\Delta^{\pm}$ and Δ_γ before the critical field. As shown in section 3 since they behave differently under exact discrete symmetries of the system, we expect that these crossings will survive beyond perturbation theory. If however the magnetic field is no longer in a high-symmetry position these symmetries are broken and one should see only avoided crossings.

3. Lanczös results

We have performed a Lanczös study of the Hamiltonian (2.1) on chains of lengths $N = 4$, 6, 8, 10, 12, 14 and 16. For a generic orientation of the magnetic field, there are no symmetries available apart from translational symmetry to reduce the size of the problem. Thus many iterations were required to obtain the first few excited levels. The energies of the ground state (in the subspace $K = 0$) and the three low-lying levels (in the subspace $K = \pi$) have been obtained with a typical precision of 10^{-6}. For a generic orientation of the magnetic field, the size of the complex Hermitian matrix $\mathcal{H}$, 3^N, is reduced by translational symmetry to $\sim 3^N/N$. The size of the Hilbert space for $N = 16$ is $\sim 1.3 \times 10^6$. On one Cray-2 processor, acting with $\mathcal{H}$ on a vector takes about 17 s and the precision of 10^{-6} is reached for ~ 60 iterations.

We have followed the triplet splitting as a function of the E term. NS experiments [19] have shown that there is a small splitting of the two low-lying modes in the case of NENP: $\Delta_x \simeq 1.05$ meV and $\Delta_y \simeq 1.25$ meV. This means that the E term is much smaller than the D term in equation (2.1) since $\Delta_z \simeq 2.5$ meV. We treat it perturbatively but keep the D term in the unperturbed Hamiltonian to be solved by the Lanczös technique. When $E = 0$ the Haldane triplet is split into a high-energy singlet and a doublet. First-order perturbation

theory for the E term requires its matrix elements in the subspace spanned by the doublet. We find a linear splitting:

$$\Delta_x = \Delta_0(D) + \kappa_0(D)E$$
$$\Delta_y = \Delta_0(D) - \kappa_0(D)E. \tag{3.1}$$

Here $\Delta_0(D)$ is the doublet gap when $E = 0$. It can be found from equation (2.11). The constant $\kappa_0(D)$ has been computed for all lattice sizes. Its values as a function of D are given in figure 1. We have used the Shanks algorithm [17] to obtain an estimate of the thermodynamic limit value of κ. In the case of NENP it has been shown [17] that the exchange coupling J is close to 44 K and $D \simeq 0.18$ J. For such values we find in the thermodynamic limit $\kappa_0 \simeq 2$. The corresponding estimate for the in-plane anisotropy is $E \simeq 0.012$ J, thus reproducing the splittings of NENP [9]. These values are used in all figures.

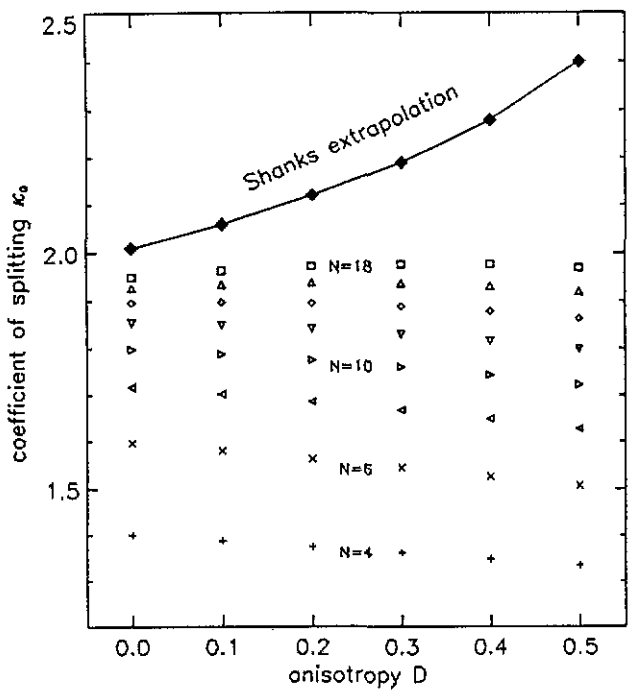

Figure 1. The coefficient κ_0 as a function of the anisotropy D up to $D = 0.5$. The raw data coming from the finite chain calculation are plotted as open symbols: from bottom to top, $N = 4$, 6, 8, 10, 12, 14, 16, and 18. We have performed an extrapolation to the thermodynamic limit using the Shanks algorithm. The corresponding results are plotted as filled diamonds.

We now take for granted the zero-field splittings and add a magnetic field along the coordinate axis. We present the Lanczös results for the longest chain we were able to deal with in figures 2–6. We find that the numerical points are very well reproduced for all chain lengths by the following procedure: we take the zero-field gaps as inputs in the perturbative formula (2.14) and obtain the field behaviour. The results are plotted as full curves in figures 2–6. One has of course to vary the gaps with the chain length but the

hyperbolic behaviour holds for *all* lengths. The deviations between the exact results and the perturbative curves are of the order of 10^{-2}. In figures 2, 3 and 4 the field lies respectively along Z, X, and Y. One of the gaps is barely affected and the other two are split according to the simple formula (2.14). If $\boldsymbol{H}$ lies along Z there is a crossing between the Δ_z and Δ_x modes (figure 2), if $\boldsymbol{H}$ lies along Y then there is a crossing between Δ_x and Δ_y (figure 4).

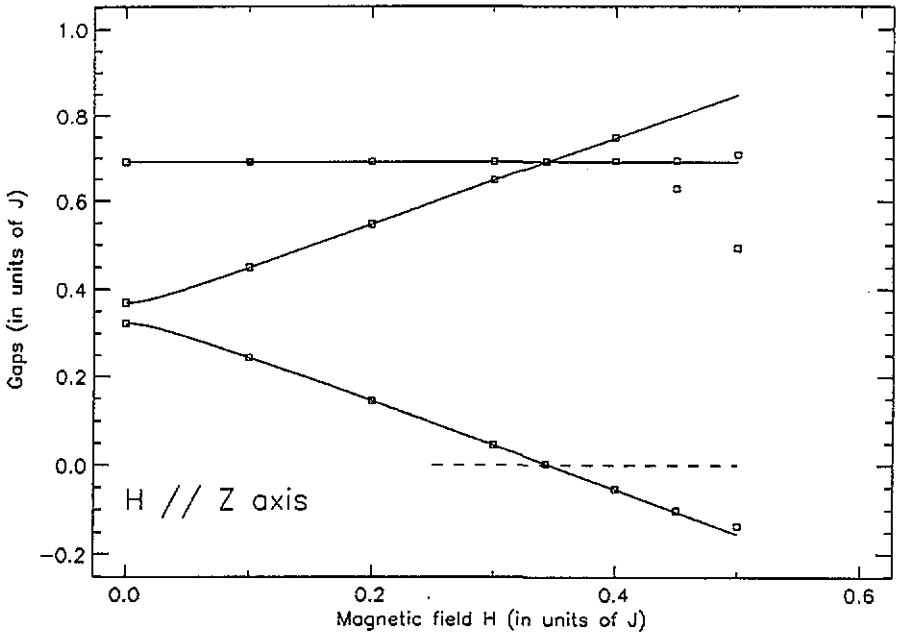

Figure 2. The three gaps in units of J as function of the magnetic field applied along the Z axis. The points are results from the Lanczös technique for a 16-spin chain. The full curves are the results of perturbation theory equation (2.14). Note the crossing between the x and z modes. The two points on the right that deviate seriously from the perturbative curves are in fact the energies of a state that do not belong to the Haldane triplet and that has crossed the upper members of the triplet. For the triplet state the deviations always stay small. The anisotropies are chosen to fit the NENP gaps: $D = 0.18$ and $E = 0.012$ in all figures.

It is interesting to note that, before the critical field is reached, one observes that other states with higher spin begin to arrive from higher energies. This is seen in all our figures: the upper 'triplet' mode always follows the perturbative trend but there are new states that are lower in energy close to H_c that do not belong to the Haldane triplet. These states will ultimately cross the ground state after the transition point [20].

Let us consider the case of figure 2 where $\boldsymbol{H}$ lies along Z. Then the operation R_z^π is a symmetry operation of the Hamiltonian. We can classify the triplet members according to their behaviour under R_z^π:

$$\begin{aligned} R_z^\pi|z\rangle &= +|z\rangle \\ R_z^\pi|x\rangle &= -|x\rangle \\ R_z^\pi|y\rangle &= -|y\rangle. \end{aligned} \tag{3.2}$$

Thus no matrix element can avoid the crossing between these two members of the triplet (x and z). It is important to realize the following: when $\boldsymbol{H} = 0$ and $\mathcal{H}_S = 0$ we can

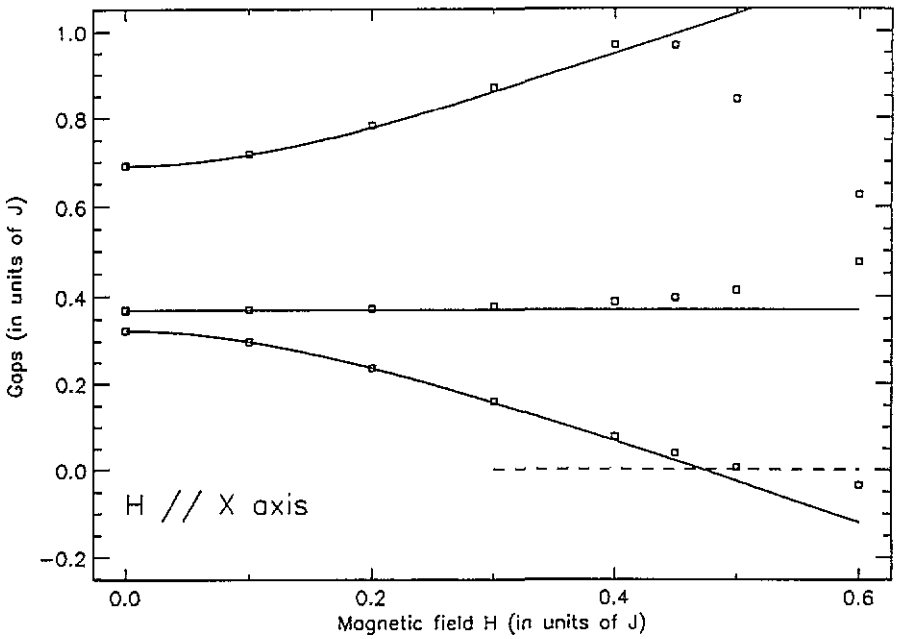

Figure 3. The three gaps in units of J as a function of the magnetic field applied along the X axis. The symbols have the same meaning as in figure 2. There is no crossing of levels before the critical field.

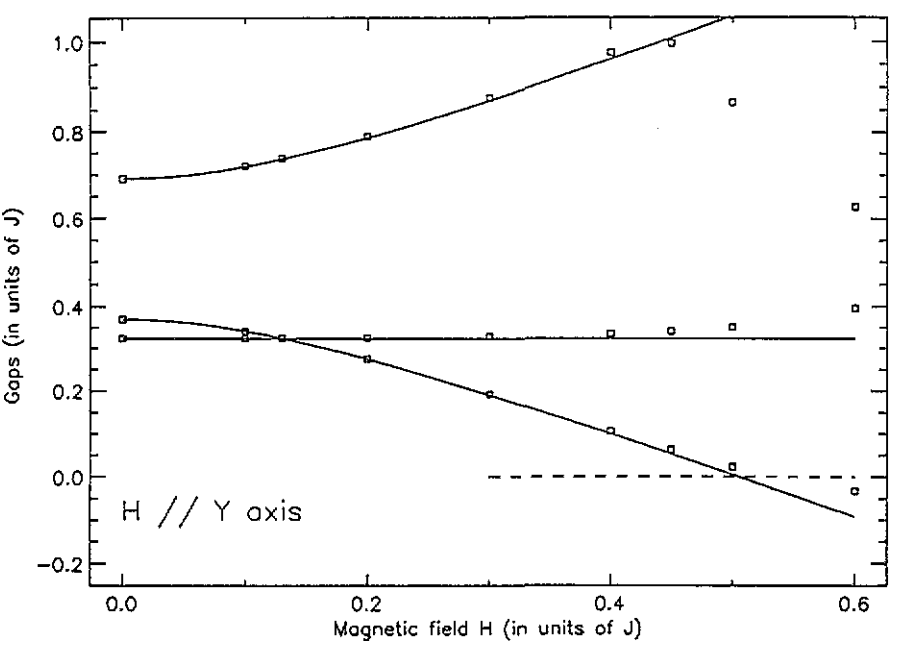

Figure 4. The three gaps in units of J as function of the magnetic field applied along the Y axis. The symbols have the same meaning as in figure 2. Note the crossing between the x and y modes.

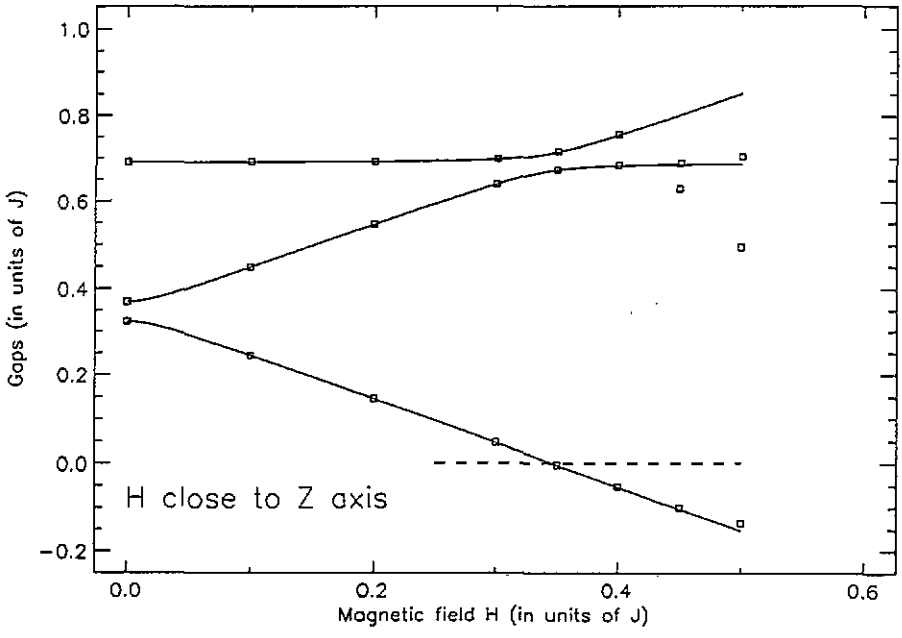

Figure 5. The three gaps in units of J as function of the magnetic field applied along a direction close to the Z axis, defined by polar angles $\theta = 5°$ and $\phi = 45°$. There is now an *avoided crossing between z and x modes since there is no longer a discrete symmetry to allow* a degeneracy. This is generic behaviour since the field is not in a symmetry plane.

demonstrate (3.2) for the degenerate triplet. By continuity the behaviour under the preserved symmetry operations R_α^π will survive the addition of $\boldsymbol{H}$ and $\mathcal{H}_S$. This does not rely upon perturbation theory but rather on the continuity of a discrete quantum number as a function of field and anisotropy. This reasoning holds also for X and Y axes.

When the field no longer lies along a coordinate axis, the crossings are avoided. A typical example is given in figure 5. Here the field is very close to the Z axis and thus there is an avoided crossing between the upper mode (z) and the intermediate (x) mode. This should be compared with figure 2 ($\boldsymbol{H} \parallel Z$). The full curves in figure 5 are obtained from the diagonalization of perturbation (2.13). It is always very close to our Lanczös results. We have checked that for various field arrangements the same property is true. Another example is given in figure 6 where the field lies close to the Y axis.

Experimental results have been reproduced by use of a formula from the effective fermionic theory [14]. The agreement of ESR [10, 11] and neutron measurements [9] is indeed very good. We note that for the $K = \pi$ mode this formula from [14] is simply our perturbation result equation (2.14), as can be seen by straightforward algebra. This means that NENP (at least) follows extremely well the hyperbolic behaviour (2.14). What we have shown is that a spin-1 chain follows the hyperbolic behaviour (2.14) by an *ab initio* Lanczös study. As a consequence the compound NENP is satisfactory described by an anisotropic spin 1, at least as far as ESR and NS are concerned.

4. Conclusion

We have studied the magnetic-field behaviour of a realistic spin-1 chain with the most

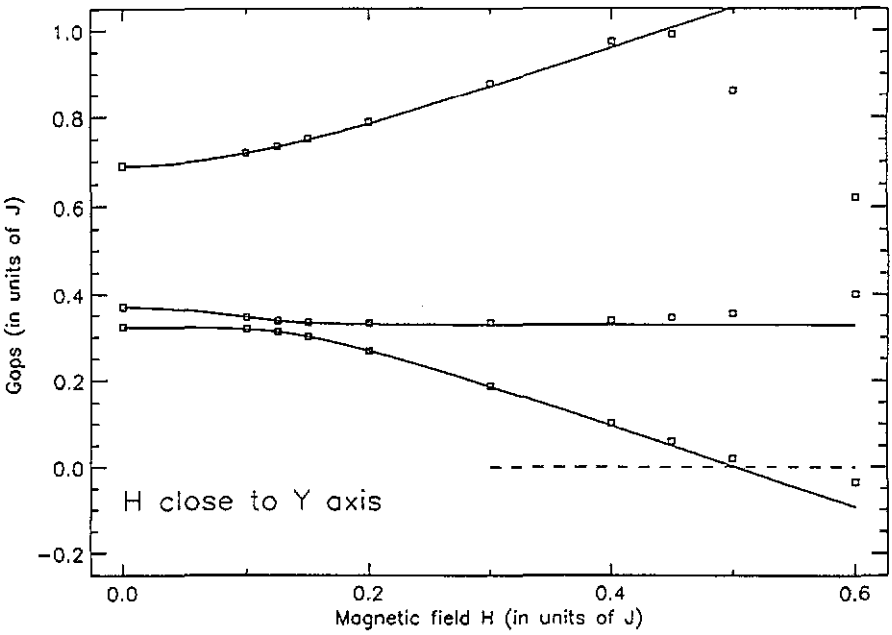

Figure 6. The three gaps in units of J as function of the magnetic field applied along a direction close to the Y axis ($\theta = 85°$ and $\phi = 80°$). The avoided crossing takes place between x and y modes.

general single-ion anisotropy that has proved adequate for NENP. The three gaps have been computed as a function of the field by means of a Lanczös technique for chains of lengths up to 16 spins. Our results are well reproduced by a simple perturbation theory. This perturbative approximation is identical to the result of the fermionic effective theory [14] when $K = \pi$. We have shown that one needs only to know first-order perturbation theory to derive it in a satisfactory manner. For arbitrary field orientation and arbitrary chain length we have observed that the perturbative behaviour holds. We thus infer that the thermodynamic limit will be also described by the same approximation. Our *ab initio* results confirm some aspects of the effective theories that have been applied to the spin-1 chain.

The field splitting of the Haldane gaps in figures 2, 3 and 4 is that found in experiments on NENP [7–11]. Both ESR and NS experiments have observed the same splitting of the Haldane gap. Below the critical field there is clearly a very good agreement between theory and experiments. At large field the asymptotic behaviour of the wavefunctions leads to a polarization of the modes that is similar to experimental data. Quantitative fits of experimental results have been performed using a hyperbolic behaviour equation (2.14). We have shown that this behaviour is obeyed by an anisotropic spin-1 chain. As a consequence the compound NENP is satisfactorily described by such a spin chain.

In the future it would be interesting to obtain the magnetization curves in a realistic spin-1 chain following the lines of [20]. Another possibility would be to investigate in detail the dynamical properties under a field as has been done recently in the zero-field case [21, 22].

Appendix

In this appendix we give for the convenience of the reader the complete perturbative formulas for the gaps. The matrix to be diagonalized is given in equation (2.13). Its characteristic polynomial is

$$X^3 + a_1 X^2 + a_2 X + a_3 = 0$$

where we have defined

$$a_1 = -(p_x + p_y + p_z)$$

$$a_2 = p_x p_y + p_y p_z + p_x p_z - (H_x^2 + H_y^2 + H_z^2)$$

$$a_3 = p_x H_x^2 + p_y H_y^2 + p_z H_z^2 - p_x p_y p_z.$$

The general solution is obtained through textbook formulas:

$$Q = \tfrac{1}{9}(a_1^2 - 3a_2) \qquad R = \tfrac{1}{54}(2a_1^3 - 9a_1 a_2 + 27a_3) \qquad T = \arccos(R/Q^{3/2}).$$

The gaps are then

$$\begin{pmatrix} G_1 \\ G_2 \\ G_3 \end{pmatrix} = -2\sqrt{Q}\begin{pmatrix} \cos(T/3) \\ \cos(T/3 + 2\pi/3) \\ \cos(T/3 + 4\pi/3) \end{pmatrix} - \frac{1}{3}a_1.$$

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[16] There are also discrete symmetries when the magnetic field lies in one of the planes (X, Y), (Y, Z), or (X, Z). They are operations involving time reversal and a discrete rotation. This is seen easily when the Y component of H is zero: the Hamiltonian expressed in the basis of eigenstates of S_i^z is then a *real* symmetric matrix. Complex conjugation (time reversal) is thus a discrete symmetry. In fact complex conjugation changes the sign of the operators S_i^y and is a symmetry when $H_y = 0$ (in this particular

basis). When the magnetic field is in another plane the system is still invariant under a combined operation involving complex conjugation and a rotation R_α^π. If, for example, $H_z = 0$ then time reversal will transform $H_y S_i^y$ into $-H_y S_i^y$ and then one uses R_x^π to return to the original Hamiltonian.

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