and  $\tilde{k}$ -space forms (as a consequence of the short-ranged correlations), it is unclear whether or not such behavior should be built into the scaling function  $\mathfrak{D}(\kappa r, 0)$  (which strictly speaking describes only the limit  $\kappa \to 0, \ r \to \infty$ ) or its analog in  $\tilde{k}$  space. The evidence on this point (Ref. 15) is ambiguously negative. The Fisher-Burford approximant, in any case, does not contain an energy-density singularity. See also M. E. Fisher and J. S. Langer, Phys. Rev. Letters 20, 665 (1968).

<sup>31</sup>D. S. Ritchie and M. E. Fisher, Phys. Rev. B 5, 2668 (1972), Table XXI. Note that the Ising values of  $G_o$  and  $\varphi$  quoted in Ref. 31 differ from and supersede those given in Table XIII of Ref. 13.

<sup>32</sup>K. G. Wilson, Phys. Rev. B <u>4</u>, 3174 (1971); <u>4</u>, 3184 (1971).

 $^{33}$ When small perturbations *do* change the symmetry, then there may still be an experimentally defined "outer critical region" within which universal critical behavior is observed. See also Ref. 11.

 $^{34}$ It is not our purpose here to give a critical review of the experimental situation. A comprehensive review of fluid behavior from this point of view has been given by M. Vincentini-Missoni, J. M. H. Levelt Sengers, and M. S. Green, Phys. Rev. Letters 22, 389 (1969); J. Res. Natl. Bur. Std. (U. S.) <u>73A</u>, 563 (1969). A similar analysis including magnetic data is given by M. Vincentini-Missoni *et al.*, Phys. Rev. B <u>1</u>, 2312 (1970). When apparently similar materials have different critical exponents, we must conclude that (i) universality fails, (ii) there are subtle symmetry differences, (iii) physical effects such as gravity, coupling to the lattice, etc., are complicating the analysis, or (iv) the true critical region has not been attained.

<sup>35</sup>From an experimentalist's point of view this is somewhat of an oversimplification in that it is only the *critical* parts of all quantities that are predicted. Sufficient data must be taken to subtract out noncritical background contributions.

<sup>36</sup>Reference 17, Eq. (3.6). Our notation parallels Ref. 17, although, as pointed out in the text, our statement of universality is not restricted to models differing by lattice type alone.

 $^{37}$ We are indebted to D. Stauffer for this observation and much of the following discussion.

<sup>38</sup>This hypothesis and the consequent relation (5.10) have now been tested *directly* for a variety of systems by D. Stauffer, M. Ferer, and Michael Wortis, Phys. Rev. Letters <u>29</u>, 345 (1972). We take this opportunity to note the following misprints in their Ref. 38: In Table I  $Y=6.0\pm0.4$  for CO<sub>2</sub>. In the footnotes to Table I,  ${}^{b}C_{sq}/R$ =  $(2/\pi)$ ... and  ${}^{k}\alpha = 0.0\pm0.03$ . In their Ref. 11,  $\chi_{0}=0.1$  in H<sub>2</sub>O and  $\eta(H_{2}O)/\eta(CO_{2}) \approx \frac{1}{2}$ .

<sup>39</sup> M. Ferer, M. A. Moore, and Michael Wortis, Phys. Rev. B <u>4</u>, 3954 (1971).

## PHYSICAL REVIEW B

## VOLUME 6, NUMBER 9

1 NOVEMBER 1972

## Energy Spectrum of the Anisotropic Magnetic Chain

Hans C. Fogedby and H. Højgaard Jensen

Physics Laboratory I, H. C. Ørsted Institute, University of Copenhagen, Copenhagen, Denmark (Received 25 January 1972)

The energy spectrum of the lowest (one-cluster) multiplet of the linear anisotropic spin- $\frac{1}{2}$  ferromagnetic chain is obtained analytically in the absence of transverse mean exchange  $(j^x+j^y=0)$  and neglecting coupling to other states. In the limit where the external field tends to zero, the semi-infinite discrete spectrum exhibits an algebraic singularity of order  $\frac{2}{3}$  as a function of the field, and an algebraic singularity as a function of the transverse anisotropy parameter  $[j^a = \frac{1}{2}(j^x - j^y)]$  of order  $\frac{1}{3}$ . At zero field the spectrum is bounded and continuous. In the high-field limit the system approaches the Ising model. A magnetic excitation spectrum of that character has recently been observed by Torrance and Tinkham in the magnetic salt CoCl<sub>2</sub> • 2H<sub>2</sub>O.

The recent observations by Torrance and Tinkham<sup>1-3</sup> of a magnon bound-state spectrum in the magnetic salt  $CoCl_2 \cdot 2H_2O$  have led to renewed interest in the dynamical properties of the linear anisotropic ferromagnetic chain. In the Torrance and Tinkham<sup>1-3</sup> notation, the system is described by the following spin- $\frac{1}{2}$  nearest-neighbor Hamiltonian:

$$\Im C = -2 \sum_{i=1}^{N} \left[ j^{z} S_{i}^{z} S_{i+1}^{z} + \frac{1}{2} j^{\perp} (S_{i}^{+} S_{i+1}^{-} + \text{H. c.}) + \frac{1}{2} j^{a} (S_{i}^{+} S_{i+1}^{+} + \text{H. c.}) \right] + \gamma H_{0} \sum_{i=0}^{N} S_{i}^{z} . \quad (1)$$

These authors investigated the magnetic excitation spectrum of (1) in detail and solved numerically the secular problem which arises from treating the mean exchange characterized by  $j^{\perp}$  and the anisotropy characterized by  $j^{a}$ , as perturbations on the Ising model characterized by the  $j^{a}$  term and the Zeeman term in (1).

In a previous article,<sup>4</sup> referred to as I, one of the present authors computed the transverse and longitudinal magnetic susceptibility to second order in  $j^a$  and  $j^{\perp}$ , and considered the zero-field limit of the transverse susceptibility in the absence of  $j^{\perp}$  and for the lowest series of energy levels.

In the present article we show that in the case  $j^{\perp}=0$ , the energy spectrum of the lowest series of levels (the one-cluster multiplet) can be derived analytically, if coupling to other states is neglected. These excitations, incidentally, are the ones observed by Torrance and Tinkham.<sup>1,2</sup> Their nu-

merical solution, which also neglects coupling to other states, is in excellent agreement with the experimental results.

The basic physics of the anisotropic magnetic chain as observed in a ferromagnetic resonance experiment arises from the symmetry-breaking  $j^a$  term in (1), which, especially at low field, induces strong transitions between the nearly degenerate Ising levels characterized by the  $j^a$  term and the Zeeman term in (1). For the present purposes it is therefore sufficient to consider the truncated Hamiltonian

$$\Im C' = -2 \sum_{i=1}^{N} \left[ j^{z} S_{i}^{z} S_{i+1}^{z} + \frac{1}{2} j^{a} (S_{i}^{+} S_{i+1}^{+} + \text{H. c.}) \right] + \gamma H_{0} \sum_{i=1}^{N} S_{i}^{z} .$$
(2)

In order to solve the eigenvalue equation  $\mathcal{K}'\Psi$ =  $E\Psi$ , the Ising model with applied field

$$\Re_{0}^{\prime} = -2 \sum_{i=1}^{N} j^{z} S_{i}^{z} S_{i+1}^{z} + \gamma H_{0} \sum_{i=1}^{N} S_{i}^{z}$$
(3)

is chosen as the unperturbed Hamiltonian. The lowest series of eigenstates of (3), corresponding to a single cluster of *n* adjacent spin deviations, with respect to the aligned ferromagnetic ground state  $| 0 \rangle$ , have the energies  $E_n^0 = 2j^z + n\gamma H_0$ ,  $n = 1, 2, \ldots, N$  and are characterized by the Bloch functions

$$\Psi_{n}^{0}(k) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \exp\left\{ik\left[x_{i} + \frac{1}{2}(n-1)a\right]\right\} \times S_{i}^{*}S_{i+1}^{*} \cdots S_{i+n-1}^{*} \mid 0\rangle, \quad (4)$$

which form an orthonormal set provided  $\langle 0|0\rangle = 1$ . Here, *a* is the interatomic distance, *N* is the total number of spins, and the angular wave number *k* runs over the first Brillouin zone,  $-\pi/a < k \le \pi/a$ . The matrix elements of the perturbing Hamiltonian

$$\mathcal{H}_{a}^{\prime} = -2 \sum_{i=1}^{N} \frac{1}{2} j^{a} (S_{i}^{*} S_{i+1}^{*} + \mathrm{H. c.})$$
(5)

between the Bloch states (4) are

$$\langle \Psi_n^{0^*}(k) \left| \Im \mathcal{C}'_a \right| \Psi_{n'}^0(k') \rangle = \delta_{kk'} \delta_{n,n'*} (-2j^a) \cos ka .$$
 (6)

Neglecting coupling to states with zero or more than one spin clusters [see Eqs. (1)-(4)], we can expand the eigenstates  $\Psi$  on the set  $\Psi_n^0$ ,

$$\Psi = \sum_{n=1}^{N} c_n \Psi_n^0(k) ,$$

and using (6), we obtain the following recursion formula for the expansion coefficients  $c_n$ :

$$n\gamma H_0 c_n - (2j^a \cos ka) (c_{n+2} + c_{n-2}) = (E - 2j^z) c_n .$$
 (7)

The states for even and odd *n*, respectively, are decoupled. For  $N \rightarrow \infty$  we obtain the boundary condition  $c_{-1}=0$  for the odd states and the condition  $c_0=0$  for the even states.

The dimensionless parameter characterizing the

eigenvalue problem is  $\eta = j^a/\gamma H_0$ . Consequently, perturbation theory in  $j^a$  is equivalent to an asymptotic expansion in  $1/\gamma H_0$ , i.e., valid at high field. In the limit of an infinite field, one obtains the result  $c_{n'} = A\delta_{nn'}$  for  $E = E_n^0$ , i.e., the Ising model. At lower field, i.e., for  $\eta > 1$ , perturbation theory ceases to be useful. In the zero-field limit, however, the eigenvalue problem (7) can be solved trivially. The bounded and continuous energy spectrum is given by

$$E=2j^{z}-4j^{a}\cos ka\cos \lambda,$$

where the quantum number  $\lambda$  runs through the interval  $0 - \frac{1}{2}\pi$ . For odd states the expansion coefficients satisfying the appropriate boundary conditions are given by  $c_n^{\text{odd}} = A \sin[\frac{1}{2}\lambda(n+1)]$ ; for the even states by  $c_n^{\text{even}} = A \sin[\frac{1}{2}\lambda n]$ . We notice incidentally that the evaluation in I of the uniform zerofield transverse magnetic susceptibility,

$$\chi_{\perp}(z) = 2/\left\{ (z - 2j^z) + \left[ (z - 2j^z)^2 - (4j^a)^2 \right]^{1/2} \right\},$$
(8)

corroborates the above result in the case of the odd states.  $\chi_1(z)$  has a branch cut corresponding to a bounded continuous energy spectrum from  $-4j^a + 2j^z$  to  $4j^a + 2j^z$ .

An exact solution of the eigenvalue problem is obtained by noticing that (7) is a recursion formula satisfied by solutions to the Bessel equation.<sup>5</sup> The Bessel function has the correct high-field behavior, and we obtain for  $j^a \cos ka > 0$ 

$$c_n = A J_{[n-(E-2j^{Z})/\gamma H_0]/2} (2j^a \cos ka / \gamma H_0).$$
(9)

For  $j^a \cos ka < 0$  we get

$$c_{n} = (-1)^{(n-1)/2} A J_{[n-(E-2j^{z})/\gamma H_{0}]/2} (|2j^{a} \cos ka|/\gamma H_{0})$$
(10)

for the odd states, and

$$c_{n} = (-1)^{n/2} A J_{[n(E-2j^{2})/\gamma H_{0}]/2} \left( \left| 2j^{a} \cos ka \right| / \gamma H_{0} \right) \quad (11)$$

for the even states. The boundary conditions are in both cases given by

 $J_{[-1-(E^{\text{odd}}-2j^{z})/\gamma H_{0}]/2}(|2j^{a}\cos ka|/\gamma H_{0})=0$ (12)

for the odd states and

$$J_{[-(E^{\text{even}}-2j^{z})/\gamma H_{0}]/2}(|2j^{a}\cos ka|/\gamma H_{0})=0$$
(13)

for the even states. We notice that  $E^{\text{odd}} = E^{\text{even}} - \gamma H_0$ .

Equations (9)-(13) provide a complete solution of the problem in terms of tabulated functions. The eigenfunctions are given by Eqs. (9)-(11), and the energy spectra of even and odd states are given by Eqs. (12) and (13), respectively. Jahnke and Emde<sup>6</sup> have plotted the zeros of the Bessel function  $J_{\nu}(x)$  as a function of order  $\nu$  and argument x from which one directly can read off the energy spectra.

As discussed above, the high-field limit of the energy spectrum can be obtained as an asymptotic



FIG. 1. Even energy levels, with corresponding unperturbed Ising levels, plotted as functions of the magnetic field.

series in  $1/\gamma H_0$  simply by doing ordinary perturbation theory in  $j^a$ . From the properties of the Bessel function, we conclude that the energy spectrum for any nonvanishing value of the magnetic field is discrete. In the limit of zero field, the infinite discrete spectrum collapses to a bounded continuous spectrum. This limit, which evidently is very singular, can be investigated by performing a double asymptotic expansion in both order and argument of the Bessel functions in (10) and (11). From Courant and Hilbert<sup>5</sup> we extract the appropriate asymptotic expansion

$$J_{\mu}(a\mu) = (2/\pi\mu \tan \alpha)^{1/2} \left\{ \cos[\mu (\tan \alpha - \alpha) - \frac{1}{4}\pi] \right\}$$

<sup>1</sup>J. B. Torrance, Jr., Ph.D. thesis (Harvard University, 1968) (unpublished); Harvard University, Division of Engineering and Applied Physics, Technical Report No. 1, 1969 (unpublished).

$$+ O(\mu^{-1/5})$$
, (14)

where  $a = 1/\cos \alpha$ ,  $0 < \alpha < \frac{1}{2}\pi$ . Setting

$$E^{\text{even}} = 2j^z - 4 \left| j^a \cos ka \right| \cos \lambda$$

and using (14) together with the boundary condition (13), we get

$$a = \frac{4 |j^a \cos ka|}{2j^z - E} = \frac{1}{\cos \lambda} = \frac{1}{\cos \alpha}$$

i.e.,  $\alpha = \lambda$ . The zeros of the Bessel function in (13) are given by the condition

$$\sin\lambda - \lambda \cos\lambda = \pi \left(\nu + \frac{3}{4}\right) \gamma H_0 / 2 \left| j^a \cos ka \right| , \qquad (15)$$

where  $\nu = 0, 1, 2...$ 

For a given value of the discrete quantum number  $\nu$ , the corresponding energy level approaches  $2j^z - 4|j^a|\cos ka|$  as  $H_0$  tends to zero. Expanding the energy around the lower band edge we get

$$E^{\text{even}} = 2j^{z} - 4 \left| j^{a} \cos ka \right| + 2 \left| j^{a} \cos ka \right| \\ \times \left[ 3\pi (\nu + \frac{3}{4}) \gamma H_{0} / 2 \left| j^{a} \cos ka \right| \right]^{2/3}.$$
(16)

Since  $dE/dH_0 \sim H_0^{-1/3}$ , we conclude that the discrete energy spectrum emerges from the lower edge of the zero-field continuum with infinite slope. The energy spectrum has an algebraic singularity at vanishing field of order  $\frac{2}{3}$ , and an algebraic singularity as a function of the coupling strength  $j^a$ , of order  $\frac{1}{3}$ .

We have plotted some of the even energy levels together with the corresponding unperturbed Ising levels as functions of the magnetic field (see Fig. 1). The odd levels are obtained from the relation  $E^{\text{odd}} = E^{\text{even}} - \gamma H_0$ .

We wish to acknowledge useful conversations with Dr. V. Emery.

<sup>3</sup>See Ref. 2, p. 595.

<sup>4</sup>Hans C. Fogedby, Phys. Rev. B <u>5</u>, 1941 (1972). <sup>5</sup>R. Courant and D. Hilbert, *Methods of Mathematical* 

Physics (Interscience, New York, 1966). <sup>6</sup>E. Jahnke and F. Emde, Tables of Functions with

Formulae and Curves (Dover, New York, 1945).

<sup>&</sup>lt;sup>2</sup>J. B. Torrance, Jr. and M. Tinkham, Phys. Rev. <u>187</u>, 587 (1969).