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1994 J. Phys.: Condens. Matter 6 3411

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# Magnetic properties of a transverse spin-1 Ising model with random crystal-field interactions

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Received 1 December 1993

Abstract. We study the phase diagram and magnetic properties of a transverse spin-1 Ising model with random longitudinal crystal-field interactions using an expansion technique for cluster identities of spin-1 localized spin systems. Partially ordered phases appear for a particular two-valued distribution  $P(D_t) = \frac{1}{2} [\delta(D_i - (1 + \alpha)D) + \delta(D_i - (1 - \alpha)D)]$ , and sufficiently small transverse field  $\Omega$ . The longitudinal and transverse magnetizations and the quadrupolar moments are calculated. General formulae, applicable to structures with arbitrary coordination number N, are given.

#### 1. Introduction

Spin systems are widespread in very different fields of physics, e.g. in the theory of magnetism, superconductivity, nuclear physics, etc. Special methods of theoretical physics are needed to describe such systems, since the commutation relations for spin components differ from the corresponding relations in both Bose and Fermi systems. The study of phase transitions in the Ising and the Heisenberg models has been the subject of much interest [1-7]. Phase diagrams of such models show various types of multicritical phenomena [3,4,7]. The Ising model in the presence of a transverse field serves for the study of cooperative phenomena and phase transitions in many physical systems [8-10]. The diluted threedimensional spin-1 Ising model with crystal-field interactions has been studied by Saber [11] within the finite-cluster approximation. The spin-1 Ising model with a random crystal field has been studied by Benyoussef et al [12] and Boccara et al [13] within the meanfield solution. Our aim is to study the influence of the transverse magnetic field on the phase diagram and magnetic properties of the spin-1 Ising model with random crystal-field interactions. We use the finite-cluster approximation [14, 15] with an expansion technique for cluster identities of spin-1 localized spin systems established by Ez-Zahraouy et al [16]. The phase diagram for coordination number N = 6 is represented in the T- $\Omega$ -D space for a fixed value of  $\alpha$ , where T,  $\Omega$  and D are respectively temperature, transverse field and longitudinal crystal field. General formulae of the magnetizations and quadrupolar moments are determined for an arbitrary coordination number N. The dependence of longitudinal and transverse magnetizations on the crystal field for several values of the transverse field and on temperature for several values of the crystal field are calculated for N = 6.

In section 2 we give the method and we calculate the state equations. Section 3 is reserved for results and discussion.

#### 2. Finite-cluster approximation

We consider a spin-1 Ising system in a simple cubic lattice described by a Hamiltonian corresponding to a paramagnet of the longitudinal-axis type in a transverse magnetic field:

$$H = -\sum_{\langle ij\rangle} J_{ij} S_{iz} S_{jz} - \Omega \sum_{i} S_{ix} + \sum_{i} D_i S_{iz}^2.$$
(1)

Here  $S_{ix}$  and  $S_{iz}$  are respectively the x component and the z component of spin-1 operator at site i;  $\Omega$  represents the transverse field;  $J_{ij}$  is the exchange interaction between spins at sites i and j, and in this paper  $J_{ij}$  is constant and equal to J;  $\langle ij \rangle$  runs over all nearest-neighbour pairs of spins; and  $D_i$  is the random crystal field governed by the probability distribution law given by:

$$P(D_i) = \frac{1}{2} [\delta(D_i - (1+\alpha)D) + \delta(D_i - (1-\alpha)D)].$$

Using a single-site cluster approximation in which attention is focused on a cluster comprising just a single selected spin labelled 0, and the neighbouring spins with which it directly interacts, the Hamiltonian containing 0 is written as

$$H_0 = AS_{0z} + BS_{0x} + D_0 S_{0z}^2 \tag{2}$$

where

$$A = -J\theta \qquad B = -\Omega \tag{3}$$

with

$$\theta = \sum_{j=1}^{N} S_{jz}.$$

This single-site Hamiltonian can readily be diagonalized and its eigenvalues and eigenvectors found. The three eigenvectors corresponding to the eigenvalues

$$\lambda_k = 2(D_0 + \rho^{1/3} \cos \phi_k)/3 \tag{4}$$

with

$$\phi_k = \frac{1}{3}\cos^{-1}(-27q/2\rho) + 2(k-1)\pi/3$$
(5)

$$o = (3\sqrt{3}/2)(27q^2 + |4p^3 + 27q^2|)^{1/2}$$
(6)

$$p = -(A^2 + B^2) - D_0^2/3 \qquad q = -D_0(2A^2 + 2/9D_0^2 + B^2)/3 \tag{7}$$

are

$$|\Psi\rangle_k = \alpha_k |+\rangle + \beta_k |-\rangle + \gamma_k |0\rangle \tag{8}$$

with

$$\alpha_k = \frac{|B(\lambda_k - D_0 + A)|}{\sqrt{2} \{B^2[(\lambda_k - D_0)^2 + A^2] + [(\lambda_k - D_0)^2 - A^2]^2\}^{1/2}}$$
(9)

$$\beta_k = \frac{\lambda_k - D_0 - A}{\lambda_k - D_0 + A} \alpha_k \qquad \gamma_k = \frac{\sqrt{2}}{B} (\lambda_k - D_0 - A) \alpha_k \tag{10}$$

in a representation in which  $S_{0z}$  is diagonal. The starting point of the single-site cluster approximation is a set of formal identities of the type

$$\langle\langle S_{0\alpha}^{p}\rangle_{c}\rangle = \left\langle \frac{\operatorname{trace}_{0}[S_{0\alpha}^{p}\exp(-\beta H_{0})]}{\operatorname{trace}_{0}[\exp(-\beta H_{0})]}\right\rangle \qquad (p = 1, 2; \ \alpha = x, z).$$
(11)

Here  $S_{0\alpha}^{p}$  is the  $\alpha$  component of the spin operator  $S_0$  raised to the power p;  $(S_{0\alpha}^{p})_c$  denotes the mean value of  $S_{0\alpha}^{p}$  for a given configuration c of all other spins, i.e. when all other spins  $S_i$  ( $i \neq 0$ ) have fixed values;  $\langle \ldots \rangle$  denotes the average over all spin configurations; trace<sub>0</sub> means the trace performed over  $S_0$  only; and  $\beta = 1/k_BT$ , T being the absolute temperature and  $k_B$  the Boltzmann constant. The equations (11) are not exact for an Ising system in a transverse field, but they have, nevertheless, been accepted as a reasonable starting point in many studies of that system [17]. Let  $\langle S_{0\alpha} \rangle_c^{\pm}$  and  $\langle S_{0\alpha}^2 \rangle_c^{\pm}$  denote respectively the mean value of  $S_{0\alpha}$  and  $S_{0\alpha}^2$  for a fixed configuration  $\pm$  of the random crystal field and for a given configuration c for all other spins.

To calculate  $\langle S_{0\alpha} \rangle_c^{\pm}$  and  $\langle S_{0\alpha}^2 \rangle_c^{\pm}$ , one has to effect the inner traces in equations (11) over the states of the spin 0, and this is most easily performed using the eigenstates of equation (8) as the basis states. In this way, it follows, on setting p = 1 and 2 in equations (11), that

$$\langle S_{0z} \rangle_{c}^{\pm} = \sum_{k=1}^{3} [(\alpha_{k}^{\pm})^{2} - (\beta_{k}^{\pm})^{2}] \exp(-\beta \lambda_{k}^{\pm}) / \sum_{k=1}^{3} \exp(-\beta \lambda_{k}^{\pm})$$
(12)

$$\langle S_{0x} \rangle_c^{\pm} = \sqrt{2} \sum_{k=1}^3 (\alpha_k^{\pm} + \beta_k^{\pm}) \gamma_k^{\pm} \exp(-\beta \lambda_k^{\pm}) / \sum_{k=1}^3 \exp(-\beta \lambda_k^{\pm})$$
(13)

$$\langle S_{0z}^2 \rangle_c^{\pm} = \sum_{k=1}^3 [(\alpha_k^{\pm})^2 + (\beta_k^{\pm})^2] \exp(-\beta \lambda_k^{\pm}) / \sum_{k=1}^3 \exp(-\beta \lambda_k^{\pm})$$
(14)

$$\langle S_{0x}^2 \rangle_c^{\pm} = \sum_{k=1}^3 \left[ (\alpha_k^{\pm} + \beta_k^{\pm})^2 / 2 + (\gamma_k^{\pm})^2 \right] \exp(-\beta \lambda_k^{\pm}) / \sum_{k=1}^3 \exp(-\beta \lambda_k^{\pm})$$
(15)

where

$$\alpha_k^{\pm} = \alpha_k \qquad \beta_k^{\pm} = \beta_k \qquad \gamma_k^{\pm} = \gamma_k \qquad \lambda_k^{\pm} = \lambda_k \qquad \text{when } D_0 = (1 \pm \alpha)D$$

The magnetizations  $m_{\alpha}$  ( $\alpha = z, x$ ) and the quadrupolar moments  $q_{\alpha}$  ( $\alpha = z, x$ ) are given by:

$$m_{\alpha} = \langle f_{\alpha}(\theta) \rangle \qquad q_{\alpha} = \langle g_{\alpha}(\theta) \rangle$$

with

$$f_{\alpha}(\theta) = \frac{1}{2} \left( \langle S_{0\alpha} \rangle_c^+ + \langle S_{0\alpha} \rangle_c^- \right) \tag{16}$$

$$g_{\alpha}(\theta) = \frac{1}{2} \left( \langle S_{0\alpha}^2 \rangle_c^+ + \langle S_{0\alpha}^2 \rangle_c^- \right)$$
(17)

where  $\langle ... \rangle$  denotes the average over all configurations of the spins  $S_{jz}$   $(j \neq 0)$ . To calculate  $\langle f_{\alpha}(\theta) \rangle$  and  $\langle g_{\alpha}(\theta) \rangle$  we have used the expansion technique for spin-1 Ising systems as follows [14].

Suppose one considers the general product  $\prod_{i=1}^{N} (\sum_{p_1=0}^{2} S_{iz}^{p_1})$ , which contains  $3^N$  terms. From these terms one may collect together all those terms containing p factors of  $S_{iz}^2$  and q factors of  $S_{iz}$ . Such a group is to be denoted by  $\{S_z^2, S_z\}_{N,p,q}$ . For example, if N = 4, p = 1 and q = 2, then

$$\{S_{z}^{2}, S_{z}\}_{4,1,2} = S_{1z}^{2}(S_{2z}S_{3z} + S_{2z}S_{4z} + S_{3z}S_{4z}) + S_{2z}^{2}(S_{1z}S_{3z} + S_{1z}S_{4z} + S_{3z}S_{4z}) + S_{3z}^{2}(S_{1z}S_{2z} + S_{1z}S_{4z} + S_{2z}S_{4z}) + S_{4z}^{2}(S_{1z}S_{2z} + S_{1z}S_{3z} + S_{2z}S_{3z}).$$
(18)

Our aim is to expand the functions of equations (16) and (17) in terms of these  $\{S_z^2, S_z\}_{N,p,q}$ . Thus, if one writes

$$f_{\alpha}\left(\sum_{i=1}^{N} S_{iz}\right) = \sum_{q=0}^{N} \sum_{p=0}^{N-q} A_{pq}^{(\alpha)}(N) \{S_{z}^{2}, S_{z}\}_{N,p,q}$$
(19)

$$g_{\alpha}\left(\sum_{i=1}^{N} S_{iz}\right) = \sum_{q=0}^{N} \sum_{p=0}^{N-q} B_{pq}^{(\alpha)}(N) \{S_{z}^{2}, S_{z}\}_{N,p,q}$$
(20)

the problem is to find the coefficients  $A_{pq}^{(\alpha)}(N)$  and  $B_{pq}^{(\alpha)}(N)$ . To achieve this, it is advantageous to transform the spin-1 system to a spin-1/2 representation containing the Pauli operators  $\sigma_{iz} = \pm 1$ . This may be accomplished by setting  $S_{iz} = \tau_{iz}\sigma_{iz}$  with  $\tau_{iz} = 0, 1$ . In this representation, equations (19) and (20) become

$$f_{\alpha}\left(\sum_{i=1}^{N}\tau_{iz}\sigma_{iz}\right) = \sum_{q=0}^{N}\sum_{p=0}^{N-q}A_{pq}^{(\alpha)}(N)\{\tau_{z},\tau_{z}\sigma_{z}\}_{N,p,q}$$
(21)

$$g_{\alpha}\left(\sum_{i=1}^{N}\tau_{iz}\sigma_{iz}\right) = \sum_{q=0}^{N}\sum_{p=0}^{N-q}B_{pq}^{(\alpha)}(N)\{\tau_{z},\tau_{z}\sigma_{z}\}_{N,p,q}$$
(22)

and must hold for arbitrary choices of  $\tau_{iz}$ . Suppose one now chooses the first r out of the N operators  $\tau_{iz}$  to be unity, and the remainder zero. Then equations (21) and (22) give

$$f_{\alpha}\left(\sum_{i=1}^{r}\sigma_{iz}\right) = \sum_{q=0}^{r}\sum_{p=0}^{r-q}A_{pq}^{(\alpha)}(N)C_{p}^{r-q}\{\sigma_{z}\}_{r,q}$$
(23)

$$g_{\alpha}\left(\sum_{i=1}^{r}\sigma_{iz}\right) = \sum_{q=0}^{r}\sum_{p=0}^{r-q} B_{pq}^{(\alpha)}(N) C_{p}^{r-q} \{\sigma_{z}\}_{r,q}$$
(24)

where  $\{\sigma_z\}_{r,q}$  is the sum of all possible products of q spin operators  $\sigma_{iz}$  out of a maximum of r, and the  $C_n^m$  are the binomial coefficients m!/n!(m-n)!. That is,

$$f_{\alpha}\left(\sum_{i=1}^{r}\sigma_{iz}\right) = \sum_{q=0}^{r} b_{q}^{(\alpha)}(r) \{\sigma_{z}\}_{r,q}$$

$$\tag{25}$$

$$g_{\alpha}\left(\sum_{i=1}^{r}\sigma_{iz}\right) = \sum_{q=0}^{r}d_{q}^{(\alpha)}(r)\{\sigma_{z}\}_{r,q}$$

$$\tag{26}$$

with

$$b_q^{(\alpha)}(r) = \sum_{p=0}^{r-q} A_{pq}^{(\alpha)}(N) C_p^{r-q}$$
(27)

$$d_q^{(\alpha)}(r) = \sum_{p=0}^{r-q} B_{pq}^{(\alpha)}(N) C_p^{r-q}.$$
(28)

The spin-1 problem of equations (19) and (20) containing N spins has thus been transformed to a spin-1/2 problem containing r spins. The advantage of doing this is that it now enables one to use directly the results already established in [18] for the spin-1/2 system. It may also be noted that, whereas the coefficients  $b_q^{(\alpha)}(r)$  and  $d_q^{(\alpha)}(r)$  for the spin-1/2 problem depend on the total number of spins present, the coefficients  $A_{pq}^{(\alpha)}(N)$  and  $B_{pq}^{(\alpha)}(N)$  are in fact independent of N, as is clear from equations (27) and (28). Thus the label N is superfluous and may henceforth be dropped. This could, of course, have been inferred directly from equations (19) and (20) by setting one of the  $S_{iz}$  spins equal to its zero value throughout. Specializing the results of [18] to a single group of r spins, one has for the current problem

$$b_{q}^{(\alpha)}(r) = \frac{1}{2^{r} C_{q}^{r}} \sum_{i=0}^{r} C_{i}^{r} \varepsilon_{i}(r,q) f_{i\alpha}(r)$$
<sup>(29)</sup>

$$d_q^{(\alpha)}(r) = \frac{1}{2^r C_q^r} \sum_{i=0}^r C_i^r \varepsilon_i(r, q) g_{i\alpha}(r)$$
(30)

where

$$\varepsilon_i(r,q) = \sum_{\mu=0}^{i} (-1)^{\mu} C^i_{\mu} C^{r-i}_{q-\mu}$$
(31)

$$f_{i\alpha}(r) = f_{\alpha}(r-2i) \tag{32}$$

$$g_{i\alpha}(r) = g_{\alpha}(r-2i). \tag{33}$$

Once the coefficients  $b_q^{(\alpha)}(r)$  and  $d_q^{(\alpha)}(r)$  have been calculated, the coefficients  $A_{pq}^{(\alpha)}$  and  $B_{pq}^{(\alpha)}$  may be found by the following procedure. First,  $A_{0q}^{(\alpha)}$  and  $B_{0q}^{(\alpha)}$  are obtained by setting r = q in equations (29) and (30). That is

$$A_{0q}^{(\alpha)} = b_q^{(\alpha)}(q) \qquad B_{0q}^{(\alpha)} = d_q^{(\alpha)}(q).$$
(34)

Then, the other  $A_{pq}^{(\alpha)}$  and  $B_{pq}^{(\alpha)}$  may be obtained by expressing equations (29) and (30) as a recurrence relation, namely as

$$A_{r-q,q}^{(\alpha)} = b_q^{(\alpha)}(r) - \sum_{p=0}^{r-q-1} A_{pq}^{(\alpha)} C_p^{r-q}$$
(35)

$$B_{r-q,q}^{(\alpha)} = d_q^{(\alpha)}(r) - \sum_{p=0}^{r-q-1} B_{pq}^{(\alpha)} C_p^{r-q}.$$
(36)

Then the magnetizations  $m_{\alpha}$  ( $\alpha = z, x$ ) and the quadrupolar moments  $q_{\alpha}$  ( $\alpha = z, x$ ) are given for an arbitrary coordination number N by

$$m_{\alpha} = \sum_{q=0}^{N} \sum_{p=0}^{N-q} A_{pq}^{(\alpha)} \langle \{S_{z}^{2}, S_{z}\}_{N, p, q} \rangle$$
(37)

$$q_{\alpha} = \sum_{q=0}^{N} \sum_{p=0}^{N-q} B_{pq}^{(\alpha)} \langle \{S_{z}^{2}, S_{z}\}_{N, p, q} \rangle.$$
(38)

Using the simplest approximation of the Zernike decoupling of the type

$$\langle S_{iz}S_{jz}\ldots S_{kz}\ldots\rangle \equiv \langle S_{iz}\rangle\langle S_{jz}\rangle\ldots\langle S_{kz}\rangle\ldots$$
 for  $i\neq j\neq k\neq\ldots$ 

and seeing that the number of elements of the group  $\{S_z^2, S_z\}_{N,p,q}$  is equal to  $C_p^N C_q^{N-p}$ , equations (37) and (38) become

$$m_{\alpha} = \sum_{q=0}^{N} \sum_{p=0}^{N-q} A_{pq}^{(\alpha)} m_{z}^{q} q_{z}^{p} C_{p}^{N} C_{q}^{N-p}$$
(39)

$$q_{\alpha} = \sum_{q=0}^{N} \sum_{p=0}^{N-q} B_{pq}^{(\alpha)} m_{z}^{q} q_{z}^{p} C_{p}^{N} C_{q}^{N-p}.$$
(40)

Let us put  $m = m_z = \langle S_z \rangle$  and  $x = q_z = \langle S_z^2 \rangle$ , and if we replace x in (39) by its expression taken from (40), we obtain an equation for m of the form

$$m = am + bm^3 + \dots \tag{41}$$

where

$$a = N \left( A_{01}^{(z)} + \sum_{p=1}^{N-1} A_{p1}^{(z)} C_p^{N-1} x_0^p \right)$$
(42)

with  $x_0$  the solution of

$$x_0 = B_{00}^{(z)} + \sum_{p=1}^N B_{p0}^{(z)} C_p^N x_0^p.$$
(43)

The critical temperature of the second-order transition is determined by a = 1. In the vicinity of a second-order transition the magnetization  $m_z$  is determined by

$$m_z^2 = (1-a)/b.$$
 (44)

At this temperature the transverse magnetization is given by

$$m_x = \sum_{p=0}^{N} B_{p0}^{(x)} C_p^N x_0^p \tag{45}$$



Figure 1. Phase diagram in  $T-\Omega-D$  space for N = 6. TCL is the tricritical line. Broken curves correspond to first-order transition.

and the quadrupolar moments  $q_{\alpha}$  ( $\alpha = z, x$ ) are given by

$$q_{\alpha} = \sum_{p=0}^{N} B_{p0}^{(\alpha)} C_{p}^{N} x_{0}^{p}.$$
(46)

The right-hand side of equation (44) must be positive. If this is not the case the transition is of first order. The point at which a = 1 and b = 0 is the tricritical point. To obtain the expression for b one has to solve (40) for small m. The solution is of the form

$$x = \dot{x}_0 + x_1 m^2 \tag{47}$$

where  $x_1$  is given by

$$x_{1} = \sum_{p=0}^{N-2} B_{p2}^{(z)} C_{2}^{N} C_{p}^{N-2} x_{0}^{p} + \sum_{p=1}^{N} p B_{p0}^{(z)} C_{p}^{N} x_{0}^{p-1} x_{1}.$$
(48)

That is

$$x_{1} = \sum_{p=0}^{N-2} B_{p2}^{(z)} C_{2}^{N} C_{p}^{N-2} x_{0}^{p} \bigg/ \bigg( 1 - \sum_{p=1}^{N} p B_{p0}^{(z)} C_{p}^{N} x_{0}^{p-1} \bigg).$$
(49)



Figure 2. (a) The crystal-field dependence of the longitudinal magnetization when T/J = 0.1. The number accompanying each curve denotes the value of  $\Omega/J$ . (b) The temperature dependence of the longitudinal magnetization when  $\Omega/J = 0.2$ . The number accompanying each curve denotes the value of D/J.

This yields

$$b = \sum_{p=0}^{N-3} A_{p3}^{(z)} C_3^N C_p^{N-3} x_0^p + N \sum_{p=1}^{N-1} p A_{p1}^{(z)} C_p^{N-1} x^{p-1} x_1.$$
(50)

### 3. Results and discussion

In this section we present results of the Hamiltonian (1) on a simple cubic lattice (N = 6).



Figure 3. (a) The crystal-field dependence of the transverse magnetization when T/J = 0.1. The number accompanying each curve denotes the value of  $\Omega/J$ . (b) The temperature dependence of the transverse magnetization when  $\Omega/J = 0.2$ . The number accompanying each curve denotes the value of D/J.

The study of the phase diagram in the  $T-\Omega-D$  space yields three different situations depending on the value of  $\alpha$  [13]; hereafter we shall consider a case ( $\alpha = 3/4$ ) in which the partially ordered phases exist. The resulting phase diagram is shown in figure 1, where on one part there exists a tricritical line (TCL) separating the surfaces of second- and first-order transitions, and on the other part there exists a first-order surface transition separating the ordered phases and the partially ordered phases; this surface exists at lower temperature and  $\Omega < \Omega_c$ . The dependences of the magnetizations  $m_z$  and  $m_x$  on the crystal field for a fixed value of the temperature (T/J = 0.1) and  $\alpha = 3/4$  are shown respectively in figures 2(a) and 3(a) for several values of the transverse field  $\Omega$ . A first-order transition is characterized by a gap in the longitudinal magnetization  $m_z$  at the crystal-field transition. Hence, for  $\Omega < \Omega_c$  and for sufficiently low temperature, in figure 2(a) (and for  $\Omega/J = 0.01$ ), we have two first-order transitions: one is from the ordered phase  $(m_r = 1)$  to the partially ordered phases  $(m_r = 1/2)$ , and the other is from the partially ordered phases to the disordered one. Such transitions are also observed in figure 3(a), in which the transverse magnetization passes through a peak for first-order transitions (figure 3(a) for  $\Omega = 0.2, 0.3, 0.5$ ) and a should r for the second-order transition. The transverse magnetization  $m_x$  increases when increasing the transverse field  $\Omega$  at low temperature, in agreement with [19], while the magnetization  $m_z$  decreases with  $\Omega$ . On the other hand, for fixed value of  $\Omega$ ,  $m_z$  decreases continuously in the vicinity of the transition temperature and vanishes at  $T = T_{\rm e}$ , for the second-order transition, and exhibits a discontinuity at the first-order transition (figure 2(b), D/J = 5.6, 5.5, 2.6). The transverse magnetization  $m_x$  increases with the strength of the crystal field at low temperature and passes through a peak for the first-order transition and a cusp for the second-order transition temperature of  $m_z$  and then falls off rapidly (see figure 3(b) as determined by the relation (45). Finally we remark that the method used here [16] allows us to see the re-entrant part observed in figure 2(b) (D/J = 5.5, 5.6); such a phenomenon is not observed within mean-field theory [13] for  $\Omega/J = 0$ .

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