

Phase Diagram of The Ising Model With Next-Nearest-Neighbour Interactions

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Abstract: We study the phase diagram of the Ising model on a Cayley tree with competing prolonged next-nearest neighbour J_p and one-level next-nearest neighbour interactions J_o . Vannimenus proved that the phase diagram of Ising model with competing nearest-neighbour interaction J_1 and prolonged next-nearest neighbour interactions J_p contains a modulated phase, as found for similar models on periodic lattices. Later Mariz *et al* generalized this result for Ising model with $J_o \neq 0$. For given lattice model on a Cayley tree, i.e., $J_p \neq 0$; $J_o \neq 0$ with $J_1 = 0$ we describe phase diagram and clarify the role of nearest-neighbour interaction J_1 and show that the class of modulated phases consists of so-called antiphase with period 4 only.

Key words: Lattice models, Cayley tree, prolonged next-nearest neighbour, one-level next-nearest neighbour, modulated phase.

INTRODUCTION

Variety of phenomena in magnetic systems has been observed in certain models with the existence of competing interactions. Systems exhibiting spatially modulated structures, commensurate or incommensurate with the underlying lattice, are of current interest in condensed matter physics (Bak, 1982). Among the idealized systems for modulated ordering, the axial next-nearest-neighbour Ising (ANNNI) model, originally introduced by Elliot (1961) to describe the sinusoidal magnetic structure of Erbium, and the chiral Potts model, introduced by Ostlund (1981) and Huse (1981) in connection with monolayers adsorbed on rectangular substrates, have been studied extensively by a variety of techniques.

A particularly interesting and powerful method is the study of modulated phases through the measure-preserving map generated by the mean-field equations, as applied by Bak (1981) and Jensen and Bak (1983) to the ANNNI model. The main drawback of the method lies in the fact that thermodynamic solutions correspond to stationary but unstable orbits. However, when these models are defined on Cayley trees, as in the case of the Ising model with competing interactions examined by Vannimenus (1981), it turns out that physically interesting solutions correspond to the attractors of the mapping comes to present. This simplifies the numerical work considerably, and detailed study of the whole phase diagram becomes feasible. Apart from the intrinsic interest attached to the study of models on trees, it is possible to argue that the results obtained on trees provide a useful guide to the more involved study of their counterparts on crystal lattices.

In the case of the Ising model with competing nearest neighbour (NN) interactions J and prolonged next-nearest neighbour interactions J_p , Vannimenus (1981) was able to find new modulated phases, in addition to the expected paramagnetic and ferromagnetic ones. From this result follows that Ising model with competing interactions on a Cayley tree is of real interest since it has many similarities with models on periodic lattices. In fact, it has many common features with them, in particular the existence of a modulated phase, and shows no sign of pathological behaviour - at least no more than mean-field theories of similar systems Vannimenus (1981). Moreover a detailed study of its properties was carried out with essentially exact results, using rather simple numerical methods. This suggests that more complicated models should be studied on trees, with the hope to discover new phases or unusual types of behaviour.

Later Mariz *et al* (1985) extended these results assuming existence also interaction J_o of the one-level

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nearest-next-neighbours. For many problems the solution on a tree is much simpler than on a regular lattice and is equivalent to the standard Bethe-Peierls theory (Katsura, 1974). Note that Wedagedera *et al* (2000) pointed out in their paper, the problem of a spin glass on a Cayley tree (or equivalently, a directed polymer) is one of a handful of models in disordered systems that can be solved exactly. Details on lattice models and their phase diagram one can find in (Kindermann, R., J.L. Snell, 1980; Mccoy, B.M., T.W. Tai, 2009; Simon, B., 2009; Wilde, E. Richard, 1998; Yeomans, J.M., 1992).

The aim of this paper is to describe phase diagram of Ising system with competing ternary and binary interactions on a Cayley tree of second order.

Definitions:

Cayley Tree A Cayley tree Γ^k of order $k \geq 1$ is an infinite tree, i.e., a graph without cycles with exactly $k+1$ edges issuing from each vertex. Let denote the Cayley tree as $\Gamma^k = (V, \Lambda)$, where V is the set of vertices of Γ^k , Λ is the set of edges of Γ^k . Two vertices x and y , $x, y \in V$ are called *nearest-neighbors* if there exists an edge $l \in \Lambda$ connecting them, which is denoted by $l = \langle x, y \rangle$. The distance $d(x, y)$, $x, y \in V$, on the Cayley tree Γ^k , is the number of edges in the shortest path from x to y .

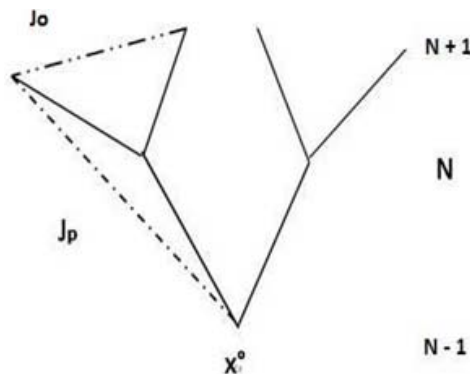


Fig. 1: Three successive generation of a Cayley tree (solid line:nearest neighbor interactions; dot-dashed line: next-nearest neighbour prolonged interactions; dot-dot-dashed line: next-nearest neighbour one-level interactions).

For a fixed $x^0 \in V$ we set

$$W_n = \{x \in V \mid d(x; x^0) = n\}, V_n = \{x \in V \mid d(x; x^0) \leq n\}$$

and L_n denotes the set of edges in V_n . The fixed vertex x^0 is called the 0-th level and the vertices in W_n are called the n -th level. For the sake of simplicity we put $|x| = d(x; x^0)$, $x \in V$. Two vertices $x, y \in V$ are called *the next-nearest-neighbors* if $d(x, y) = 2$. Two vertices x, y are called the next-nearest-neighbours if distance $d(x, y) = 2$. The next-nearest-neighbours vertices x and y are called one-level next-nearest-neighbours if x, y

$\in W_n$ for some n and is denoted by $\langle \overline{x, y} \rangle$. The next-nearest-neighbour vertices x, y that are not one-level

are called prolonged next-nearest-neighbours vertices and is denoted by $\langle \tilde{x}, \tilde{y} \rangle$. (see Fig. 1)

The Hamiltonian H will have the following form:

$$H(\sigma) = -J_p \sum_{\langle \tilde{x}, \tilde{y} \rangle} \sigma(x)\sigma(y) - J_o \sum_{\langle \overline{x, y} \rangle} \sigma(x)\sigma(y) \tag{1}$$

where first summation is over prolonged next-nearest-neighbours and second is over one-level next-nearest-neighbours. Below we study the phase diagram of Ising model (1) and compare with phase diagram of Vannimenus's model Vannimenus (1981). We consider this model on the semi-infinite Cayley tree of order

2. A semi-infinite Cayley tree of order 2, denoted by G_+^2 , is a graph without cycles, with exactly 3 edges

incident to each vertex, except a root $x^0 \in V$ which only emanates 2 edges from the vertex. Note that the Ising models with nearest-neighbour and one-level next-nearest-neighbour interactions have been studied in

(Ganikhodjaev, N.N., 2002; Ganikhodjaev, N.N., 2004; Monroe, J.L., 1992; Monroe, J.L., 1994).

Basic Equations:

We used a recurrent equation relating to partition function as the main equation to investigate the limiting behaviour of our model. To set up our basic equation in recurrence equations relating the partition function of n -generation tree to the partition functions of its subsystems; we have take into account the partial partition functions for all the possible configurations of the spins in two successive generations Vannimenus (1981).

Following the Mariz *et al* (1985) and Vannimenus (1981), for instance, we identify $Z_n(+_-)$ is the partition function of an n -generation tree where the spin in the last generation is up and the two spins in the preceding one are down. There are eight different configurations; but it is reasonable to consider only six different configuration since $Z_n(+_-)$ and $Z_n(-_+)$ are equal. For convenience, we define the following variable to write down the recurrent system:

$$\begin{aligned} z_1 &= Z_n(+_+) \\ z_2 &= Z_n(+_-) = Z_n(-_+) \\ z_3 &= Z_n(-_-) \\ z_4 &= Z_n(-_+) \\ z_5 &= Z_n(+_-) = Z_n(-_+) \\ z_6 &= Z_n(-_-) \end{aligned}$$

Let primed variables (z'_1, \dots, z'_6) correspond to the Z_{n+1} and the interactions appear through the parameters

$$c = \exp\left(\frac{2J_o}{T}\right) \text{ and } b = \exp\left(-\frac{2J_p}{T}\right)$$

It is straightforward to establish the following recursive relations (see [10]):

$$\begin{aligned} z'_1 &= \left(\sqrt{cb}z_1 + \frac{2}{\sqrt{c}}z_2 + \frac{\sqrt{c}}{b}z_3 \right)^2 \\ z'_2 &= \left(\sqrt{cb}z_1 + \frac{2}{\sqrt{c}}z_2 + \frac{\sqrt{c}}{b}z_3 \right) \left(\sqrt{cb}z_4 + \frac{2}{\sqrt{c}}z_5 + \frac{\sqrt{c}}{b}z_6 \right) \\ z'_3 &= \left(\sqrt{cb}z_4 + \frac{2}{\sqrt{c}}z_5 + \frac{\sqrt{c}}{b}z_6 \right)^2 \\ z'_4 &= \left(\frac{\sqrt{c}}{b}z_1 + \frac{2}{\sqrt{c}}z_2 + \sqrt{cb}z_3 \right)^2 \end{aligned}$$

$$z'_5 = \left(\frac{\sqrt{c}}{b} z_1 + \frac{2}{\sqrt{c}} z_2 + \sqrt{cb} z_3 \right) \left(\frac{\sqrt{c}}{b} z_4 + \frac{2}{\sqrt{c}} z_5 + \sqrt{cb} z_6 \right)$$

$$z'_6 = \left(\frac{\sqrt{c}}{b} z_4 + \frac{2}{\sqrt{c}} z_5 + \sqrt{cb} z_6 \right)^2$$

Note that $(z'_2)^2 = z'_1 z'_3$ and $(z'_3)^2 = z'_4 z'_6$ so that we can omit the equations for u_2 and u_5 . Let introduce new variable u_i with $u_i = \sqrt{z_i}$; $z_i = u_i^2$. Then the recurrence equations above are reduced to the recurrent system into four independent variables:

$$u'_1 = (b\sqrt{c}u_1^2 + \frac{2}{\sqrt{c}}u_1u_3 + \frac{\sqrt{c}}{b} u_2^2)$$

$$u'_3 = (b\sqrt{c}u_3^2 + \frac{2}{\sqrt{c}}u_4u_6 + \frac{\sqrt{c}}{b} u_6^2)$$

$$u'_4 = \left(\frac{\sqrt{c}}{b} u_1^2 + \frac{2}{\sqrt{c}}u_1u_3 + b\sqrt{c}u_3^2 \right)$$

$$u'_6 = \left(\frac{\sqrt{c}}{b} u_3^2 + \frac{2}{\sqrt{c}}u_4u_6 + b\sqrt{c}u_6^2 \right) .$$
(2)

In the paramagnetic phase (high symmetry phase) we will have $u_1 = u_6$ and $u_3 = u_4$. Thus, for analysis on phase diagram, we will reduce our variable by the following form:

$$u'_6 = \left(\frac{\sqrt{c}}{b} u_3^2 + \frac{2}{\sqrt{c}}u_4u_6 + b\sqrt{c}u_6^2 \right) .$$

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Finally we will have following recurrent equations:

$$u'_6 = \left(\frac{\sqrt{c}}{b} u_3^2 + \frac{2}{\sqrt{c}}u_4u_6 + b\sqrt{c}u_6^2 \right) .$$

$$u'_6 = \left(\frac{\sqrt{c}}{b} u_3^2 + \frac{2}{\sqrt{c}}u_4u_6 + b\sqrt{c}u_6^2 \right) .$$
(3)

$$u'_6 = \left(\frac{\sqrt{c}}{b} u_4^2 + \frac{2}{\sqrt{c}} u_4 u_6 + b\sqrt{c} u_6^2 \right) .$$

Phase Transition:

The variable x is just a measure of the frustration of the nearest-neighbour bonds. Let $(x^*, 0, 0)$ be a fixed point of the recurrence system (3), where x^* is given by

$$x^* = \frac{cb^2x^{*2} + 2bx^* + c}{b^2c + 2bx^* + cx^{*2}} . \tag{4}$$

Below we describe the solutions of equation (4). Note that for the model (1) a phase transition occurs if the equation (4) has more than one solution. Consider the equation $x = f(x)$, where

$$x^* = \frac{cb^2x^{*2} + 2bx^* + c}{b^2c + 2bx^* + cx^{*2}} . \tag{5}$$

Computing the first and second derivatives of (5), we have as below:

$$f'(x) = \frac{2c(b-1)(b+1)(b^2cx+b+bx^2+cx)}{(b^2c+2bx+cx^2)^2}$$

$$f''(x) = \frac{2c(b-1)(b+1)(b^4c^2-2bcx^3-(3c^2+2b^2c^2)x^2-6bcx-4b^2+b^2c^2)}{(b^2c+2bx+cx^2)^3} .$$

In particular, if $b < 1$, then $f(x) < 0$ and f is decreasing function. This implies that there can only be one solution of equation (4). Thus, we can restrict ourselves to the case $b > 1$; when $f(x) > 0$ and f is increasing. An inflection point x_{inf} of the function f is a solution of the equation $f(x) = 0$; i.e. $-(2bcx^3 + (3c^2+3b^2c^2)x^2+6cx + b^2(4-b^2c^2-c^2))=0$

If $4-b^2c^2-c^2 \geq 0$ then $f''(x) < 0$ and thus f is concave down or convex; hence there is only one solution of equation (4). For $4-b^2c^2-c^2 < 0$ we get definitely one inflection point and if $x < x_{inf}$ then $f''(x) > 0$; i.e., f is concave up, and if $x > x_{inf}$ then $f''(x) < 0$; i.e., f is concave down or convex. Thus there are at most three solution of equation (4). Now we find the explicit form of these solutions. By simple transformations the equation (4) is reduced to the following:

$$(x - 1) \left(x^2 - \left(b^2 - 2\frac{b}{c} - 1 \right) x + 1 \right) = 0 \tag{6}$$

From first factor of (6) we get definitely $x^*_1 = 1$ as the first fixed point. Now, we need to examine the second factor of the equation, i.e., the quadratic equation $x^2 - \left(b^2 - 2\frac{b}{c} - 1 \right) x + 1 = 0$. Simple analysis of this quadratic equation provides the following result.

Proposition

The equation (4) has single solution if $0 < b < \frac{1+\sqrt{1+3c^2}}{c}$ and has three solutions if $b \geq \frac{1+\sqrt{1+3c^2}}{c}$

Corollary:

For the model (1) a phase transition occurs if and only if $b \geq \frac{1+\sqrt{1+3c^2}}{c}$. The Figure 2 shows the domain of phase transition.

Phase Diagram:

It is convenient to know the broad features of the phase diagram before discussing the different transitions in more detail. This can be achieved numerically in a straightforward fashion. The recursion relations (3) provide us the numerically exact phase diagram in $(T/J_o, -J_p/J_o)$ space. Let $T=J_o = \alpha$ and $(-J_p/J_o) = \beta$, and respectively $c = \exp(2\alpha^1)$ and $b = \exp(-2\alpha^1\beta)$.

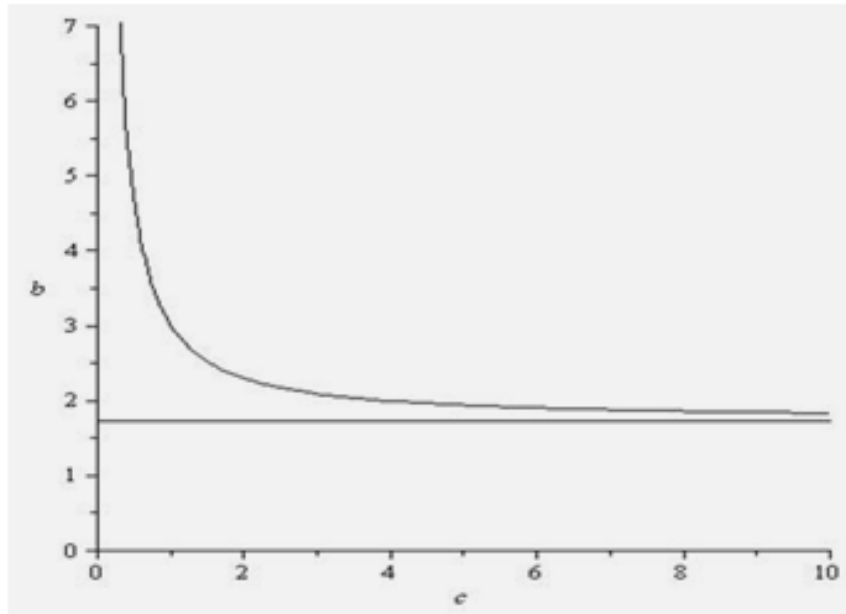


Fig. 2: The phase transition domain : graph of $b = \frac{1 + \sqrt{1 + 3c^2}}{c}$.

Starting from Initial Conditions:

$$\begin{aligned}
 x^{(1)} &= 1 \\
 y_1^{(1)} &= \frac{b^2 - 1}{b^2 + 1} \\
 y_2^{(1)} &= \frac{b^2 - 1}{b^2 + 1}
 \end{aligned} \tag{7}$$

that corresponds to boundary condition $\bar{\sigma}^{(n)} \equiv 1$ one iterates the recurrence relations (3) and observes their behavior after a large number of iterations. In the simplest situation a fixed point (x^*, y_1^*, y_2^*) is reached. It corresponds to a paramagnetic phase if $y_1^* = 0, y_2^* = 0$ or to a ferromagnetic phase if $y_1^*, y_2^* \neq 0$. Secondary, the system may be periodic with period p , where case $p = 2$ corresponds to anti-ferromagnetic phase and case $p = 4$ corresponds to so-called antiphase, that denoted $\langle 2 \rangle$ for compactness. Finally, the system may remain aperiodic.

The distinction between a truly aperiodic case and one with a very long period is difficult to make numerically. Plotting the points when the phases change from one phase to another, we got a diagram shows region for each phase exists in this model. The resultant phase diagram is shown in Figure 3.

At low temperature $T = 0$, three different ground-states are encountered: paramagnetic, anti-ferromagnetic and state with period 4: A state with period 4 is a state which the magnetization of the successive generations alternates with an anti-ferromagnetic structure $(+ + - -)$. This phase also known as antiphase $\langle 2 \rangle$.

The anti-ferromagnetic and $\langle 2 \rangle$ phases are separated by paramagnetic phase at finite temperature which extends down to T . All three phases meet at a critical point; $T = 0; \beta = 0$.

Stability of the Phases:

One finds numerically that the para-antiferro and para- $\langle 2 \rangle$ transitions are continuous. The transition lines may then be obtained by linearizing the system (3) around the fixed point $(x^*, 0, 0)$. As x^0 does not depend on y_1 and y_2 in first order, the nontrivial part of the linearization is expressed in terms of the Jacobian:

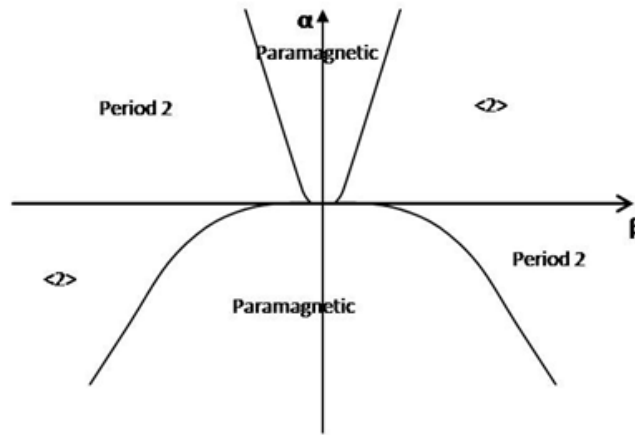


Fig. 3: Phase diagram of Ising model with NNN interactions (prolonged and one-level).

$$\begin{bmatrix} y'_1 \\ y'_2 \end{bmatrix} = \begin{bmatrix} \frac{2(b^2c + bx^*)}{b^2c + 2bx^* + cx^{*2}} & \frac{2(b + cx^*)}{b^2c + 2bx^* + cx^{*2}} \\ -\frac{2x^*(c + bx^*)}{c + 2bx^* + b^2cx^{*2}} & -\frac{2x^*(b^2cx^* + b)}{c + 2bx^* + b^2cx^{*2}} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad (8)$$

The secular equation has form

$$\lambda^2(b^2c + 2bx + cx^2)(c + 2bx + b^2cx^2) - 2\lambda(b^2c^2 + bcx + b^3cx - b^3cx - b^3cx - b^2c^2x^4 - bcx^3) - 4x(b^4c^2x + b^3cx^2 + b^3c + bc + c^2x - bcx^2) = 0 \quad (9)$$

The fixed point is linearly stable if the eigenvalues have moduli smaller than one. Two cases have to be examined, according to whether the eigenvalues are real or complex. One can see that in first quadrant ($J_p < 0$; $J_o > 0$) and third quadrant ($J_p > 0$; $J_o < 0$) there is para-<2> transition and in second ($J_p > 0$; $J_o > 0$) and fourth quadrants ($J_p < 0$; $J_o < 0$) there is anti-ferromagnetic- para transition. Since para-<2> and para-antiferromagnetic transition lines are symmetric below we consider para-<2> transition lines in first and third quadrants.

The Para-<2> Transition:

When the eigenvalue λ are complex, the fixed point is approached in an oscillatory way and the instability occurs when eigenvalue $\lambda = i$. The equation (9) becomes:

$$x^4 + \frac{2}{bc}(3b^2 - 1)x^3 + \left(-\frac{3}{b^2} + 5b^2 - \frac{4}{c^2}\right)x^2 - \frac{2}{bc}(3b^2 - 1)x + 1 = 0 \quad (10)$$

By substitution $x + \frac{1}{x} = t$, since $c^2 \sim 0$ this equation is reduced to

$$t^2 + \frac{2(3b^2 - 1)}{c}t + \frac{(5b^2 + 3)(b^2 - 1)}{b^2} = 0 \quad (11)$$

In first quadrant where $b < 1$, the transition exists only if $b^2 \leq \frac{1}{3}$ i.e., this equation has positive root $t > 2$. The equality $b^2 = \frac{1}{3}$ or $\beta = \frac{In3}{2}\alpha$ corresponds to the asymptote of the transition line in first quadrant

for large T which is in agreement with the slope obtained numerically (see Fig. 3). In third quadrant $b < 1$ and $c < 1$ so that since $c^2 \sim 0$ the equation (10) is reduced to

$$4bx^2 - 2cx + bc^2 = 0 \quad (12)$$

This equation has positive root if $b \leq \frac{1}{2}$. The equality $b = \frac{1}{2}$ or $\beta = \alpha \ln 2$ corresponds to the asymptote of the transition line in third quadrant which in agreement with the slope obtained numerically (see Fig. 3).

Discussion and Conclusion:

Consider the previous work of Vannimenus (1981). In his phase diagram at low temperature, $T = 0$, only two different ground states are encountered: the ferromagnetic state when $p < 1/3$ and a state of period 4 for $p > 1/3$ (in this project paper, we use β instead of p). His work consists of an Ising spin on a Cayley tree considering 2 bonds: nearest neighbour and next-nearest neighbour interaction which restricted to spins belonging to the same branch (prolonged). The succession of phase with increasing temperature, T is *ferro* \rightarrow *para* \rightarrow *modulated* \rightarrow *para*. Thus, based on his investigation, the phases meet at $p = 1/3$; $T = 0$ when nearest neighbour and next-nearest neighbour (prolonged) interactions are being considered.

However, based on this investigation, for competing interaction involving only the second neighbour interactions, prolonged and one-level; all phases meet at $\beta = 0$; $T = 0$. Without nearest neighbour interactions, the critical point from left and right move towards the center of the graph (see Fig. 3). This is different from Vannimenus (1981) and Mariz *et al* (1985) which their critical point similar to each other. Moreover, when we have NN and NNN interaction, there arise antiphase and modulated phase. But, if we only consider the NNN or second neighbour prolonged and one-level, among modulated phase, we only found the antiphase and anti-ferromagnetic. Without NN interaction, the phase diagram becomes more simpler than the diagram found by Vannimenus (1981).

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