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Reentrant and successive phase transitions in the Ising model with competing interactions

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The double-chain approximation is used to obtain phase diagrams for the Ising model with ferromagnetic nearest-neighbor and antiferromagnetic crossed next-nearest-neighbor interactions. Successive phase transitions are observed on three-dimensional lattices in small regions of interaction parameters where a transition from the ferromagnetic to the antiferromagnetic state occurs when the temperature is decreased. On the other hand, reentrant phenomena are observed on two-dimensional lattices.

I. INTRODUCTION

Frustrated systems have been investigated intensively in recent years. In such systems, several two-dimensional Ising models with competing interactions have been solved exactly. In some cases, reentrant phenomena are observed[1-3] which are important in connection with spin-glass transitions. One of the simplest examples is the two-dimensional Ising model solved by Vaks *et al.*,[1,4] in which a half of the diagonal next-nearest-neighbor interactions are included.

In this paper we use the double-chain approximation[5] to obtain phase diagrams for the two and three-dimensional Ising models with all the diagonal next-nearest-neighbor interactions except in the plane perpendicular to the chains. Reentrant phenomena are only observed in the two-dimensional case. In three-dimensional cases, there exist small regions of the interaction parameters where a transition from the ferromagnetic state to an antiferromagnetic state occurs when the temperature is decreased.

II. DOUBLE-CHAIN APPROXIMATION

We start with the following Hamiltonian:

$$H=-J_1\sum_{\langle ij\rangle_1}S_iS_j-J_2\sum_{\langle i,j\rangle_2}S_iS_j-J_3\sum_{\langle i,j\rangle_3}S_iS_j\ , \tag{1}$$

where $\langle i,j\rangle_1$, $\langle i,j\rangle_2$, and $\langle i,j\rangle_3$ represent intrachain nearest-neighbor pairs, interchain nearest-neighbor pairs, and interchain diagonal next-nearest-neighbor pairs, respectively. Next-nearest-neighbor interactions are not included in the plane perpendicular to the chains. We assume that $J_2\geq 2J_1/z$ and $J_3<0$, where z is the number of nearest-neighbor chains. So the antiferromagnetic ordered phase has the layered structure perpendicular to the chains and the correlations among layers can be treated effectively in the chain approximation.

The approximation[5] is formulated on a double chain described in Fig. 1. We take into account two kinds of ordered states, namely the ferromagnetic state and an antiferromagnetic state in which the magnetization is staggered along the chains but ferromagnetically ordered within each plane perpendicular to the chains. The staggered magnetization in the antiferromagnetic phase is transformed to a uniform ferromagnetic magnetization by changing the signs of J_1 and J_3. In the following discussion, the transformed ferromagnetic state is used in place of the antiferromagnetic state.

The free energy per site $f(m)$ in the approximation is given by[5]

$$\beta f(m)=\frac{z}{2}(-\ln\eta_1+2Bm)+(1-z)(-\ln\lambda_1+B^{(1)}m)\ , \tag{2}$$

where η_1 and λ_1 are the largest eigenvalues of the transfer matrices for the double chain and the single chain, respectively, and B and $B^{(1)}$ are the effective fields acting on the double chain and the single chain. B and $B^{(1)}$ are determined self-consistently to give the same magnetization. The explicitly form of η_1 is obtained analytically by solving a cubic equation in this case, and it is given by

$$\eta_1=2(-p)^{1/2}\cos\left[\frac{1}{3}\arccos\left[\frac{-q}{2(-p)^{3/2}}\right]\right]-\frac{A}{3}\ , \tag{3}$$

where

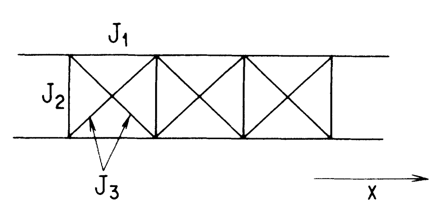

FIG. 1. Double-chain: Intrachain and interchain nearest-neighbor interactions are denoted by J_1 and J_2. J_3 represents crossed next-nearest-neighbor interactions.

$$p=\frac{3B-A^2}{9}\ ,\qquad q=\frac{2A^3-9AB+27C}{27}\ , \tag{4}$$

with

$$A=-(a+a'+d+e)\ ,$$
$$B=aa'+ad+ae+a'd+a'e-2b'^2-2b^2-c^2\ , \tag{5}$$
$$C=-aa'd-aa'e-4bb'c+2ab'^2+2a'b^2+c^2d+c^2e$$

in the expression,

$$\begin{aligned} a&=\exp(2\nu_1+\nu_2+2\nu_3+2B),\\ a'&=\exp(2\nu_1+\nu_2+2\nu_3-2B)\ ,\\ b&=\exp(B),\quad b'=\exp(-B)\ ,\\ c&=\exp(-2\nu_1+\nu_2-2\nu_3)\ ,\\ d&=\exp(2\nu_1-\nu_2-2\nu_3)\ ,\\ e&=\exp(-2\nu_1-\nu_2+2\nu_3)\ , \end{aligned} \tag{6}$$

where the notation of $\nu_i=\beta J_i$ is used. λ_1 is given by

$$\lambda_1=\exp(\nu_1)\cosh B^{(1)} +[\exp(2\nu_1)\sinh^2 B^{(1)}+\exp(-2\nu_1)]^{1/2}\ . \tag{7}$$

The magnetization can be obtained by solving the following equation:

$$\frac{\partial f(m)}{\partial m}=\frac{z}{2}(2B)+(1-z)B^{(1)}=0\ . \tag{8}$$

III. RESULTS AND DISCUSSION

Phase diagrams are obtained from (1) and (8). We give phase diagrams for $z=2$, 3, 4, and 6, which correspond to lattices described in Figs. 2(a)–2(d), respectively.

Phase diagrams for $z=2$ are shown in Figs. 3(a)–3(c) for $\alpha=1.0$, 1.01, and 2.0, where $\alpha\equiv J_2/J_1$ is the anisotropic parameter. Solid lines and dashed-lines represent

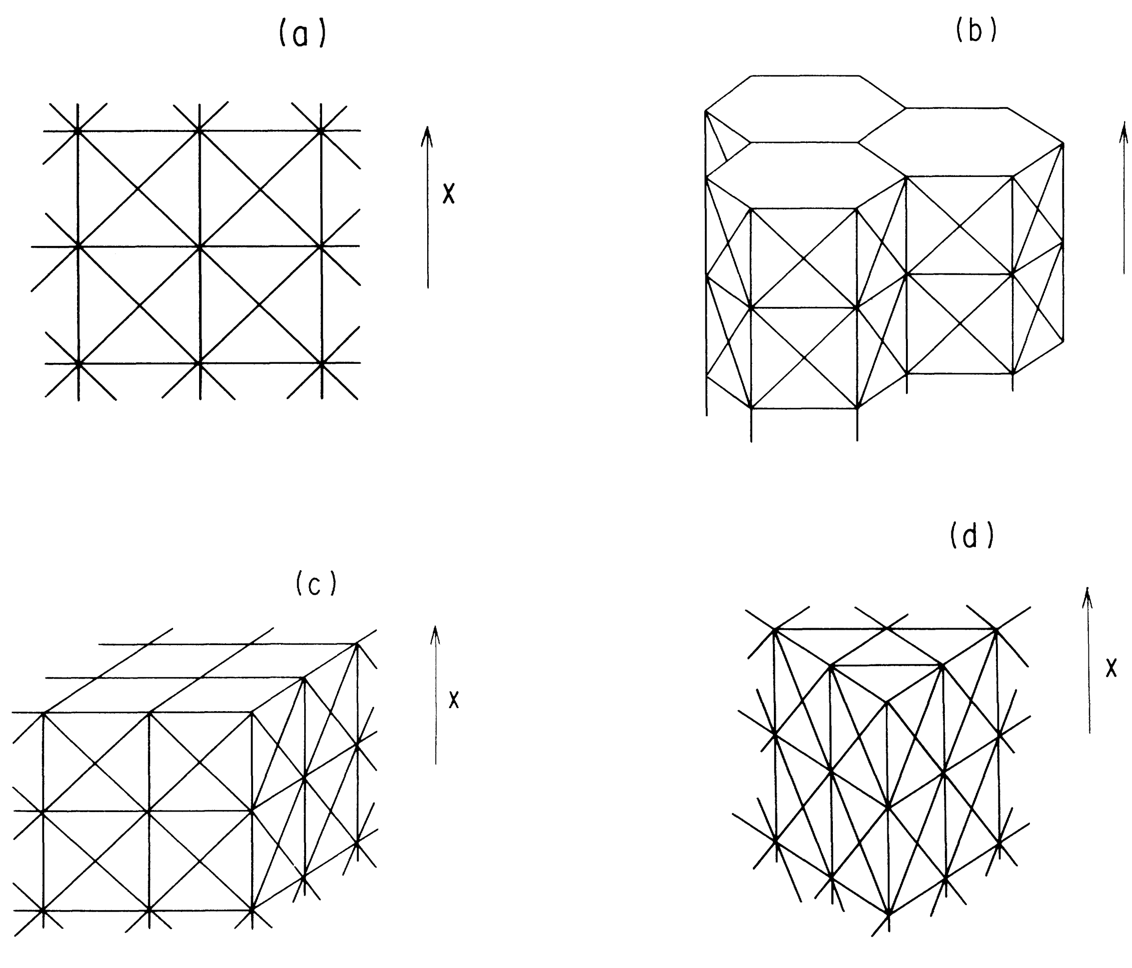

FIG. 2. (a)–(d) are lattices with described next-nearest-neighbor interactions for $z=2$, 3, 4, and 6, respectively.

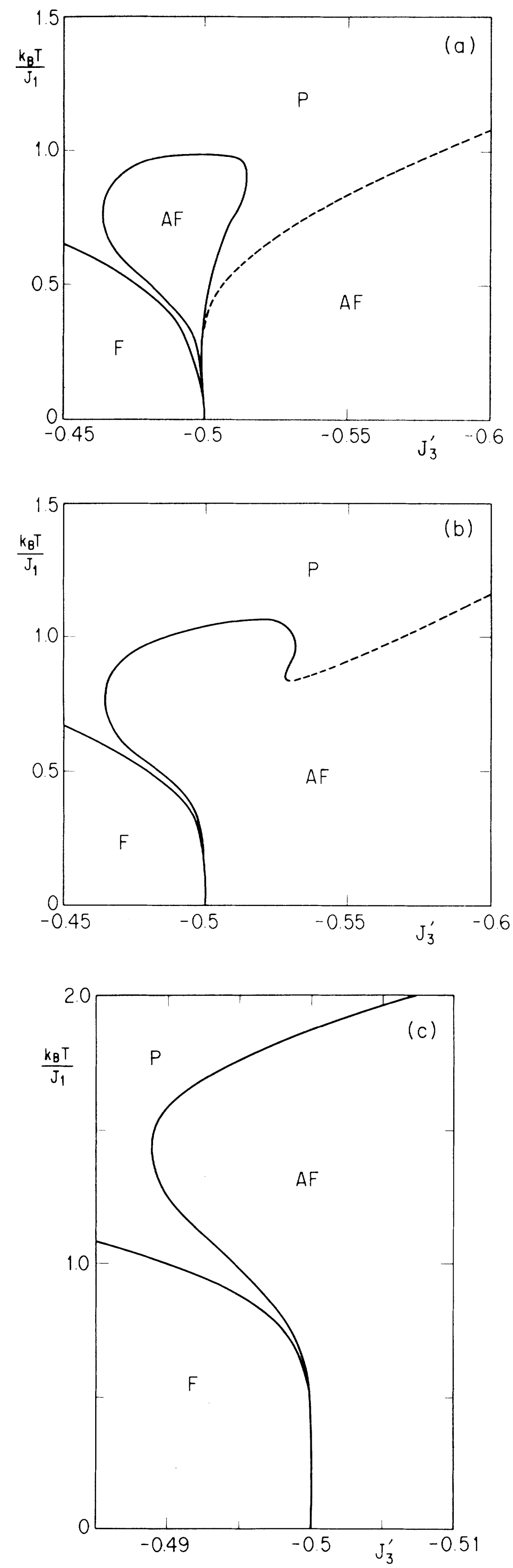

FIG. 3. Phase diagrams for $z=2$. (a)–(c) correspond to $\alpha=1.0$, 1.01, and 2.0, respectively. Solid lines and dashed lines represent second-order and first-order transitions.

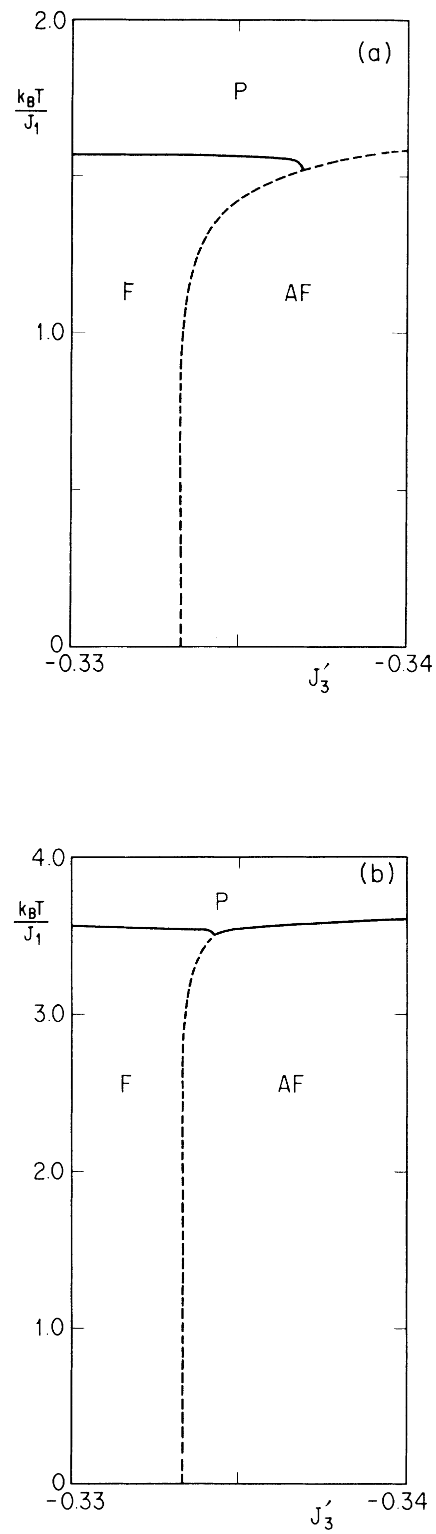

FIG. 4 Phase diagrams for $z=3$. (a) and (b) correspond to $\alpha=1.0$ and 2.0, respectively. Solid lines and dashed lines represent second-order and first-order transitions.

second-order and first-order transitions, respectively, and $J_3'=J_3/J_1$. Strange appearance of the phase diagrams for $\alpha=1.0$ and 1.01 might be an artifact caused by the anisotropic nature of the double-chain approximation. Reentrant phenomena occur in these cases for narrow ranges of J_3'. As will be discussed below, it seems essential for the occurrence of the reentrance in this model to treat the crossed next-nearest-neighbor interactions properly as well as to include the correlation along chains.

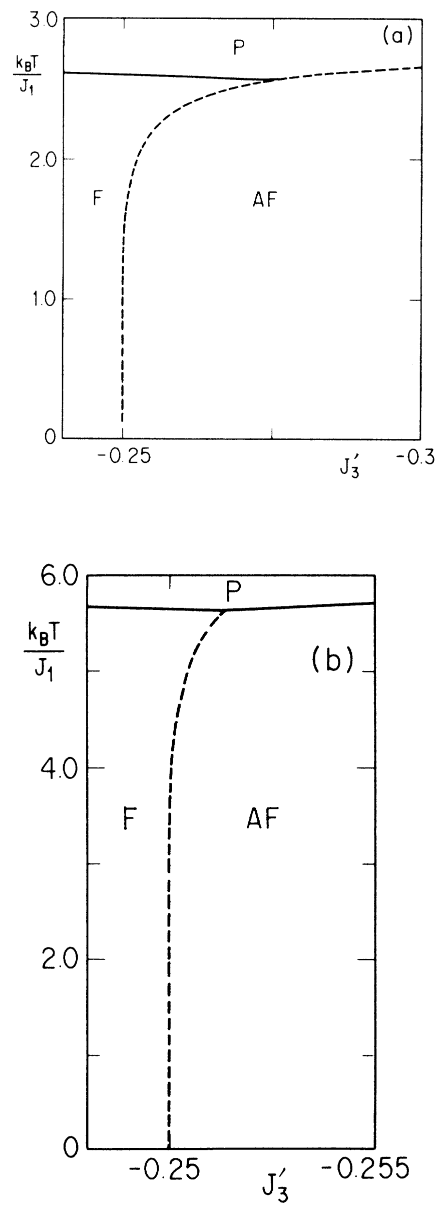

FIG. 5. Phase diagrams for $z=4$. (a) and (b) correspond to $\alpha=1.0$ and 2.0, respectively. Solid lines and dashed lines represent second-order and first-order transitions.

Phase diagrams for $z=3$ are shown in Figs. 4(a) and 4(b) for $\alpha=1.0$ and 2.0. In these cases, there exist narrow ranges of J_3' where a transition from the ferromagnetic state to the antiferromagnetic state occurs when the temperature is decreased.

Qualitative features of phase diagrams for $z=4$ and 6 are the same as those for $z=3$. Phase diagrams for $z=4$ are shown in Figs. 5(a) and 5(b) for $\alpha=1.0$ and 2.0, and a phase diagram for $z=6$ with $\alpha=1.0$ is shown in Fig. 6.

To clarify the importance of the next-nearest-neighbor interaction for the qualitative difference between the two-dimensional case and the three-dimensional cases, we investigate the model in the single-chain approximation, in which the crossed next-nearest-neighbor interactions are not treated properly although the correlation along chains are included as in the double-chain approximation. The free energy f_0 in this approximation becomes

$$\beta f_0=-\ln\lambda_1+\frac{z}{2}\nu_2 m^2+z\nu_3 m^2 , \tag{9}$$

where λ_1 is the same form as (7). In this approximation, $B^{(1)}$ is given by

$$B^{(1)}=z\nu_2 m+2z\nu_3 m . \tag{10}$$

The consistency condition to obtain the magnetization is given by

$$\frac{\exp(\nu_1)\sinh B^{(1)}}{[\exp(2\nu_1)\sinh^2 B(1)+\exp(-2\nu_1)]^{1/2}}=m . \tag{11}$$

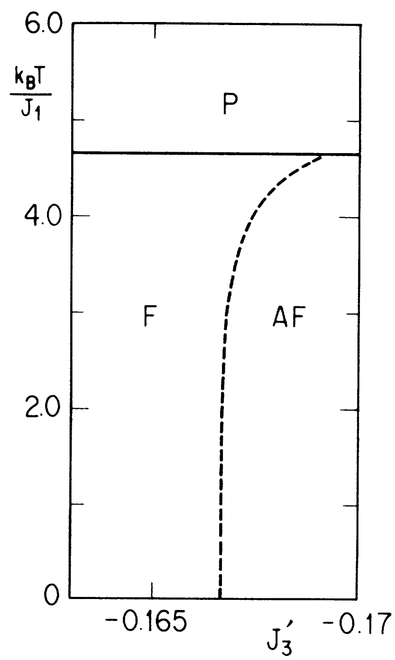

FIG. 6. Phase diagram for $z=6$ with $\alpha=1.0$. Solid lines and dashed lines represent second-order and first-order transitions.

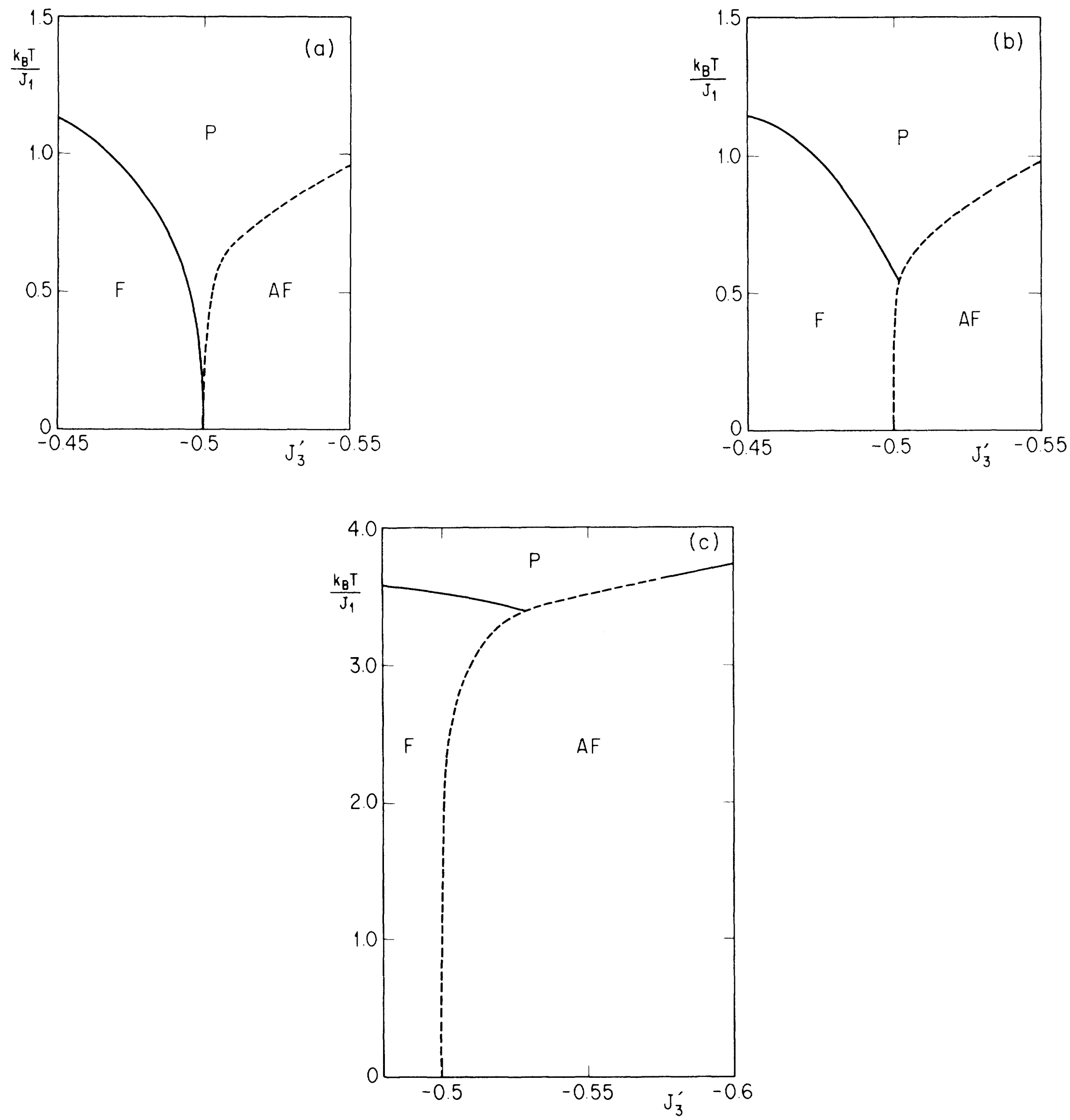

FIG. 7. Phase diagrams for $z=2$ in the single-chain approximation. (a)–(c) correspond to $\alpha=1.0$, 1.01, and 2.0, respectively. Solid lines and dashed lines represent second- and first-order transitions.

It should be noted that solutions of this equation for the same values of v_1, zv_2, and zv_3 are the same. As a consequence, phase diagrams for the same $z\alpha$'s are the same when the J_3' axis is scaled properly. In particular, no qualitative difference appears between the two- and three-dimensional cases. Examples of phase diagrams for $z=2$ are shown in Figs. 7(a)–7(c) for $\alpha=1.0$, 1.01, and 2.0, respectively.

To summarize, we have obtained phase diagrams for the Ising model with crossed next-nearest-neighbor competing interactions in the double-chain approximation. Reentrance appears only in the two-dimensional case. Successive phase transitions occur in the three-dimensional cases for small ranges of the parameters. Proper treatment of the next-nearest-neighbor interactions in an approximation is necessary to explain the qualitative difference between the two- and three-dimensional cases.

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