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Bifurcation of a periodic instanton and quantum-classical transition in the biaxial nano-ferromagnet with a magnetic field along hard axis*

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Crossover from classical to quantum regimes of the barrier transition rate in a biaxial ferromagnetic magnet with a magnetic field applied along hard anisotropy axis is investigated. We show that the type of action-temperature diagrams can be determined by counting the number of bifurcation points. The model possesses not only the known type I and II, but also the interesting type III and IV of transition which do not occur in general.

Keywords: quantum tunnelling, phase transition
PACC: 7335C, 6460, 0570F

1. Introduction

Recently, there have been intensive studies on the quantum-classical crossover of the barrier transition rate in magnetic nano-particles. The escape from a metastable state or coherent transition between two degenerate states at high temperature is dominated by classical thermal activation which follows the Arrhenins law, $\Gamma_{\rm th} \sim \exp(-\triangle U/T)$, and at zero temperature by quantum tunnelling, $\Gamma_q \sim \exp(-S)$, S being independent of temperature. At some critical temperature the crossover from the quantum to classical regime occurs, which can be viewed as a kind of phase transition. The phase transition can be first order, with a discontinuous first derivative of the action-temperature diagram at the crossover temperature, or second order, with only a jump of the second derivative in the smooth temperature-action curve.[1−3] It was demonstrated under certain assumption on the shape of potential barrier that the phase transition is second-order.[4,5] Chudnovsky,[1], however, showed that if the Euclidean oscillation period $P_0(E)$ of the instanton is a nonmonotonic function of the instanton energy E, the crossover can be the first-order phase transition. Later the sharp first-order transitions were indeed found theoretically in spin systems which are believed to be theoretical models of molecular magnet $Mn_{12}Ac$ and Fe_8.[6−13] In particular, a criterion for the first-order transition has been derived,[14] and various effective Hamiltonians of spin systems have been studied intensively.[9,14,15] It has been shown that the type of action-temperature diagram can be classified according to the numbers of bifurcation points of the period instanton.[16] Smooth second-order transition is referred to the type I in which there is no bifurcation point. The type II is a sharp first-order transition in which there is one bifurcation point and the Euclidean action-temperature curve exhibits an abrupt change at crossover from the periodic instanton to sphaleron, i.e., from quantum tunnelling(QT)

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to thermal activation(TA). Type III has two bifurcation points and the smooth second-order transition occurs between TA and thermally assisted quantum tunnelling(TAQT) near the top of barrier while with decreasing temperature sharp first-order transition occurs from TAQT to QT at the ground state, i.e., in this type, the second-order transition is followed by first-order transition.[1,17] Although the case of the magnetic field along hard anisotropy axis which leads to new quantum interference phenomenon[12,18,19] has been investigated in the context of quantum-classical transition,[15,17] in the present paper, with the help of instanton method,[20−22] we restudy the transition from quantum to classical regime for a biaxial anisotropy nano-magnet with external field along hard axis in order to explore a bifurcation of a periodic instanton in the Euclidean action-temperature diagram, and thus to understand the whole behaviour of tunnelling rate in the model. The external field along hard axis not only increases the height of barrier but also changes the barrier shape. Varying barrier shape by changing external field the model not only reproduces all the three types mentioned in Ref.[16], but also possesses the interesting type IV of transition with three bifurcation points which is named first-order crossover followed by first-order crossover in Ref.[17]. We begin with the effective semiclassical Lagrangian of the system and show the four types of transition from quantum to classical regime in terms of Euclidean action-temperature diagram.

2. Effective Lagrangian and criterion for first-order transition

Consider a biaxial single domain anisotropy magnet with XOY easy plane and the easy X axis in the XOY plane. When an external magnetic field is applied along the hard anisotropy axis (Z axis), the Hamilton operator of the model can be written as

$$\hat{H} = K_1 \hat{S}_z^2 + K_2 \hat{S}_y^2 - g\mu_{\mathrm{B}} B \hat{S}_z, \tag{1}$$

where K_1 and K_2 are the longitudinal and transverse anisotropy constants, respectively, satisfying the condition $K_1 > K_2$. With the help of spin-coherent-state path integral we obtain an effective Euclidean Lagrangian

$$L_E = \frac{1}{2} m(\phi) \left(\frac{\mathrm{d}\phi}{\mathrm{d}\tau}\right)^2 + V(\phi), \tag{2}$$

and

$$m(\phi) = \frac{1}{2K_1\left(1 - \lambda \sin^2\phi\right)}, \tag{3}$$

$$V(\phi) = K_2 S^2 \sin^2\phi \left(1 - \frac{h^2}{1 - \lambda \sin^2\phi}\right), \tag{4}$$

are the position-dependent mass and the effective potential, respectively, where ϕ is a spherical parameter of classical spin vector, S is the spin, $\lambda = K_2/K_1$ and $h = B/B_{\mathrm{c}}$ ($B_{\mathrm{c}} = 2K_1 S/g\mu_{\mathrm{B}}$). In Eq.(2) we do not retain the first derivative term since it has no contribution to the equation of motion. The tunnelling at finite E is dominated by the periodic instanton which satisfies the following equation of motion:

$$\frac{1}{2} m(\phi) \left(\frac{\mathrm{d}\phi}{\mathrm{d}\tau}\right)^2 - V(\phi) = -E. \tag{5}$$

The Euclidean action along the instanton trajectory is written as

$$S_{\mathrm{E}} = \int L_{\mathrm{E}} \mathrm{d}\tau = W(E) + EP(E), \tag{6}$$

with

$$W(E) = 2\sqrt{2} \int_{\phi^i(E)}^{\phi^f(E)} \sqrt{m(\phi)\left[V(\phi) - E\right]} \mathrm{d}\phi, \tag{7}$$

$$P(E) = \sqrt{2} \int_{\phi^i(E)}^{\phi^f(E)} \sqrt{\frac{m(\phi)}{V(\phi) - E}} \mathrm{d}\phi, \tag{8}$$

which is the period of oscillation as a function of energy E and related to temperature T by $P(E) = 1/T$. $\phi^i(E)$ and $\phi^f(E)$ are turning points. At high temperature the thermodynamic action is given by

$$S_0 = \frac{U_0}{T}, \tag{9}$$

with U_0 being the barrier height. In semiclassical approximation the transition rate at temperature T is dominated by[1]

$$\Gamma(T) \sim \mathrm{e}^{-S_{\min}(T)}, \tag{10}$$

where $S_{\min}(T)$ is actual action which goes along the minimum of these two actions (thermal and periodic instanton) and is called the optimum path. There are two criteria for the existence of first-order transition between the classical and quantum regime. The nonmonotonic behaviour of the oscillation period as a function of energy, i.e., the existence of a minimum in the P-E curve, is used as a condition for first-order phase transition.[1] When the condition is satisfied, the corresponding temperature dependence of the action has an abrupt change at some critical temperature $T = T_0^{(1)}$, i.e. the first derivative of $S_{\min}(T)$

is discontinuous. The criterion can give directly the action-temperature diagram of first-order transition from quantum to classical regime and the temperature $T_0^{(1)}$. Another criterion for the first-order transition was derived in Ref.[13] and can be used to obtain the phase boundary.

3. Phase transition with field along hard axis

The effective potential $V(\phi)$ in Eq.(4) has three different shapes depending on the field range. For the sake of convenience we study the transition of quantum to classical regime for the model in three different regions separately.

3.1. The case of $0 < h < 1 - \lambda$

The potential for $0 < h < 1 - \lambda$ is shown in Fig.1(a) and looks like a regular barrier between $\phi = 0$ and $\phi = \pi$. The turning points corresponding to energy E are

$$\phi_1^i(\varepsilon) = \arcsin\sqrt{\frac{G_1 - Q_1}{2\lambda}}, \tag{11}$$

$$\phi_1^f(\varepsilon) = \pi - \arcsin\sqrt{\frac{G_1 - Q_1}{2\lambda}}, \tag{12}$$

where $G_1 = 1 - h^2 + \lambda\varepsilon$ ($\varepsilon = E/K_2S^2$) and $Q_1 = \sqrt{G_1^2 - 4\lambda\varepsilon}$. From Eqs.(8), (6) and (7) we obtain the period of oscillation and Euclidean action as

$$P_1(\varepsilon) = \frac{g_1}{K_2 S}\mathcal{K}(k_1), \tag{13}$$

$$S_{1E}(\varepsilon) = S\Bigg\{\varepsilon g_1\mathcal{K}(k_1) - 4\sqrt{\frac{Q_1}{\lambda}}\Big[(1-\alpha_1^2)\Pi(\alpha_1^2, k_1) - (1-\bar{\alpha}_1^2)\Pi(\bar{\alpha}_1^2, k_1)\Big]\Bigg\}, \tag{14}$$

with

$$g_1 = \frac{2\sqrt{\lambda}}{\sqrt{Q_1}}, \qquad k_1^2 = \frac{1}{2}\left(1 + \frac{G_1 - 2\varepsilon}{Q_1}\right),$$

$$\alpha_1^2 = \frac{1}{2}\left(1 - \frac{G_1 - 2\lambda}{Q_1}\right),$$

$$\bar{\alpha}_1^2 = \frac{2 - Q_1 - G_1}{2(1-\lambda)}\alpha_1^2,$$

where $\mathcal{K}(k_1)$ and $\Pi(\alpha_1^2, k_1)$ are the complete elliptic integral of the first and the third kind. The corresponding thermodynamic action is

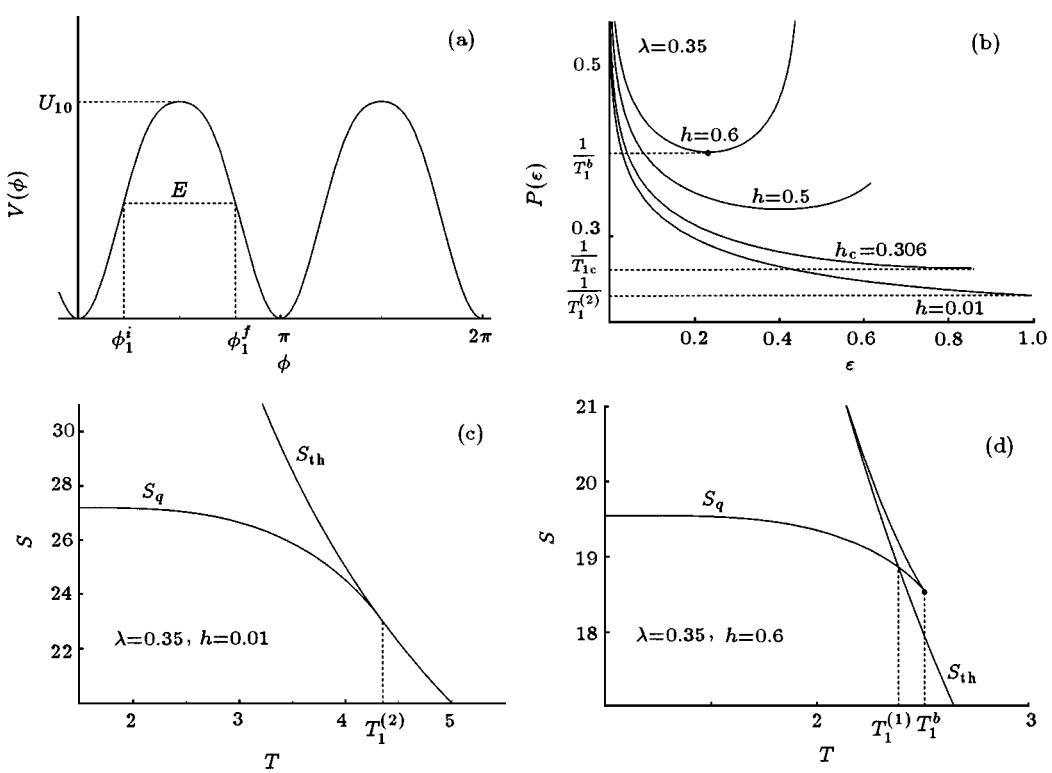


Fig.1. Potential, periods of periodic instantons and action-temperature diagrams for $\lambda = 0.35$ and $0 < h < 1-\lambda$ with $S^2 = 100$ and $K_2 = 1$. (a) Effective potential. (b) The periods of periodic instantons. (c) Type I: second-order transition (no bifurcation point). (d) Type II: first-order transition (one bifurcation point).

$$S_{10}(T) = \frac{U_{10}}{T}, \tag{15}$$

where $U_{10} = K_2 S^2\left(1 - \dfrac{h^2}{1-\lambda}\right)$. The influence of the magnetic field on the behaviour of period and the type of phase transition are shown in Figs.1(b)–(d) for $S^2 = 100, K_2 = 1$ and $\lambda = 0.35$. The period $P_1(\varepsilon)$ decreases monotonically with energy increasing for $h < h_c$ (Fig.1(b)) and corresponding action-temperature curve with smooth second-order transition at $T_1^{(2)}$ is shown in Fig.1(c) where there is no bifurcation point. When $h > h_c$ the period $P_1(\varepsilon)$ has a minimum at the point of $\dfrac{\mathrm{d}P_1}{\mathrm{d}\varepsilon} = 0$ which corresponds to the bifurcation point (corresponding temperature is T_1^b) in the action-temperature diagram. Fig.1(d) displays the behaviour of the optimum path $S_{\min}$ going along the minimum action of S_q and S_{th} with temperature decreasing. S_q and S_{th} are connected at temperature $T = T_1^{(1)}$ but their first derivative with respect to T has a jump.

3.2. The case of $1 - \lambda < h < (1-\lambda)^{1/2}$

The effective potential for $1 - \lambda < h < \sqrt{1-\lambda}$ is shown in Fig.2(a). The minimum at $\phi = \pi/2$ is a local minimum. $\phi = 0$ and $\phi = \pi$ are two degenerate ground states. Consider a trajectory $\left(\text{joining } \phi_2^i \text{ and } \pi - \phi_2^i\right)$ with the energy E such that $U_2 < E < U_{20}$ $\left(U_2 = K_2 S^2\left(1 - \dfrac{h^2}{1-\lambda}\right), U_{20} = K_2 S^2 \dfrac{(1-h)^2}{\lambda}\right)$. The trajectory consists of motion in imaginary time from ϕ_2^i to ϕ_2^f and from $\pi - \phi_2^f$ to $\pi - \phi_2^i$ and motion in real time from ϕ_2^f to $\pi - \phi_2^f$. The contribution to the Euclidean action in Eq.(10) comes from two imaginary-time parts of the trajectory, while the real-time part only affects the quantum phase interference. The turning points for given energy E are

$$\phi_2^i(\varepsilon) = \arcsin\sqrt{\frac{G_2 - Q_2}{2\lambda}}, \tag{16}$$

$$\phi_2^f(\varepsilon) = \arcsin\sqrt{\frac{G_2 + Q_2}{2\lambda}}, \tag{17}$$

with $G_2 = G_1$ and $Q_2 = Q_1$. From Eqs.(8), (6) and (7) the period of periodic instanton and Euclidean action for the trajectory considered above are obtained as

$$P_2(\varepsilon) = \frac{g_2}{K_2 S}\mathcal{K}(k_2), \tag{18}$$

$$\begin{aligned} S_{2E}(\varepsilon) =& S g_2 q_2 \left[\left(\frac{1}{\alpha_2^2} - \frac{1}{\bar{\alpha}_2^2}\right)\mathcal{K}(k_2)\right. \\ &+ \left(1 - \frac{1}{\alpha_2^2}\right)\Pi(\alpha_2^2, k_2) \\ &\left. - \left(1 - \frac{1}{\bar{\alpha}_2^2}\right)\Pi(\bar{\alpha}_2^2, k_2)\right] \\ &+ \varepsilon S g_2 \mathcal{K}(k_2), \end{aligned} \tag{19}$$

where

$$g_2 = \sqrt{\frac{8\lambda}{G_2 + Q_2 - 2\varepsilon}}, \quad k_2^2 = \frac{2Q_2}{G_2 + Q_2 - 2\varepsilon},$$

$$q_2 = \frac{2Q_2}{\lambda}, \quad \alpha_2^2 = \frac{2Q_2}{Q_2 - G_2 + 2\lambda},$$

$$\bar{\alpha}_2^2 = \frac{2(1-\lambda)}{2 - G_2 - Q_2}\alpha_2^2.$$

The corresponding thermodynamic action is

$$S_{20} = \frac{U_{20}}{T}. \tag{20}$$

For the trajectory with energy E such that $0 < E < U_2$ the period of periodic instanton and Euclidean action have the same forms as that of the case of $0 < h < 1 - \lambda$. Fig.2(b) shows the period as a function of instanton energy for $\lambda = 0.5$ and $\lambda = 0.99$. When $\lambda = 0.5$ and $h < h_c$ ($h_c = 0.618$) there is only one bifurcation point corresponding to temperature T_2^{b1} and the sharp first-order transition takes place at temperature $T = T_2^{(1)}$ (Fig.2(c)). The periodic instanton in the range of $\dfrac{\mathrm{d}P}{\mathrm{d}\varepsilon} > 0$ dose not contribute to the transition rate since there is a classical solution with the same period and lower energy. It is interesting to study the behaviour of quantum-classical transition for $h > h_c$. The competition between TA and TAQT near the top of barrier leads to the smooth second-order transition occurring at $T_2^{(2)}$ (Fig.2(d)). When $T < T_2^{(2)}$, $S_{\min}$ goes along action S_{taq} and at temperature $T = T_2^{(1)}$ sharp first-order transition appears as the result of competition between TAQT and QT. The bifurcation point corresponding to the minimum of the period is at $T = T_2^{b2}$. The other bifurcation point appearing at $T = T_2^{b3}$ is not a proper bifurcation point since the point is not a proper extremum point of period $P(\varepsilon)$, but as a common end of S_{taq} and the action corresponding to the period instanton of $\dfrac{\mathrm{d}P}{\mathrm{d}\varepsilon} > 0$, it may be called a bifurcation point. Thus Fig.2(d) gives a behaviour of type III transition, i.e. the second-order transition followed by a first-order transition. For $\lambda = 0.5$ $h_c = 0.618$ is a critical field under which the type III of quantum-classical transition occurs. $\lambda \sim 1$ is a more interesting case and not

only the type III, but also the type IV of transition appears. For $\lambda = 0.99$ and $h = 0.09$, the period as a function of instanton energy has two minima (Fig.2(b)) to which corresponding bifurcation points in the action-temperature diagram are at temperature T_2^{b4} and T_2^{b6} respectively (Fig.2(e)). With temperature decreasing, at $T = T_2^{b5}$ the third bifurcation point appears as the common end of $S_{\rm taq}$ and the action corresponding to the period instanton of $\dfrac{\mathrm{d}P}{\mathrm{d}\varepsilon} > 0$. When $T = T_{21}^{(1)}$ the first-order transition occurs. With temperature decreasing the optimum path $S_{\rm min}$ goes along $S_{\rm taq}$, and when $T = T_{22}^{(1)}$ another first-order transition takes place. Fig.2(e) displays the behaviour of the type IV of transition.

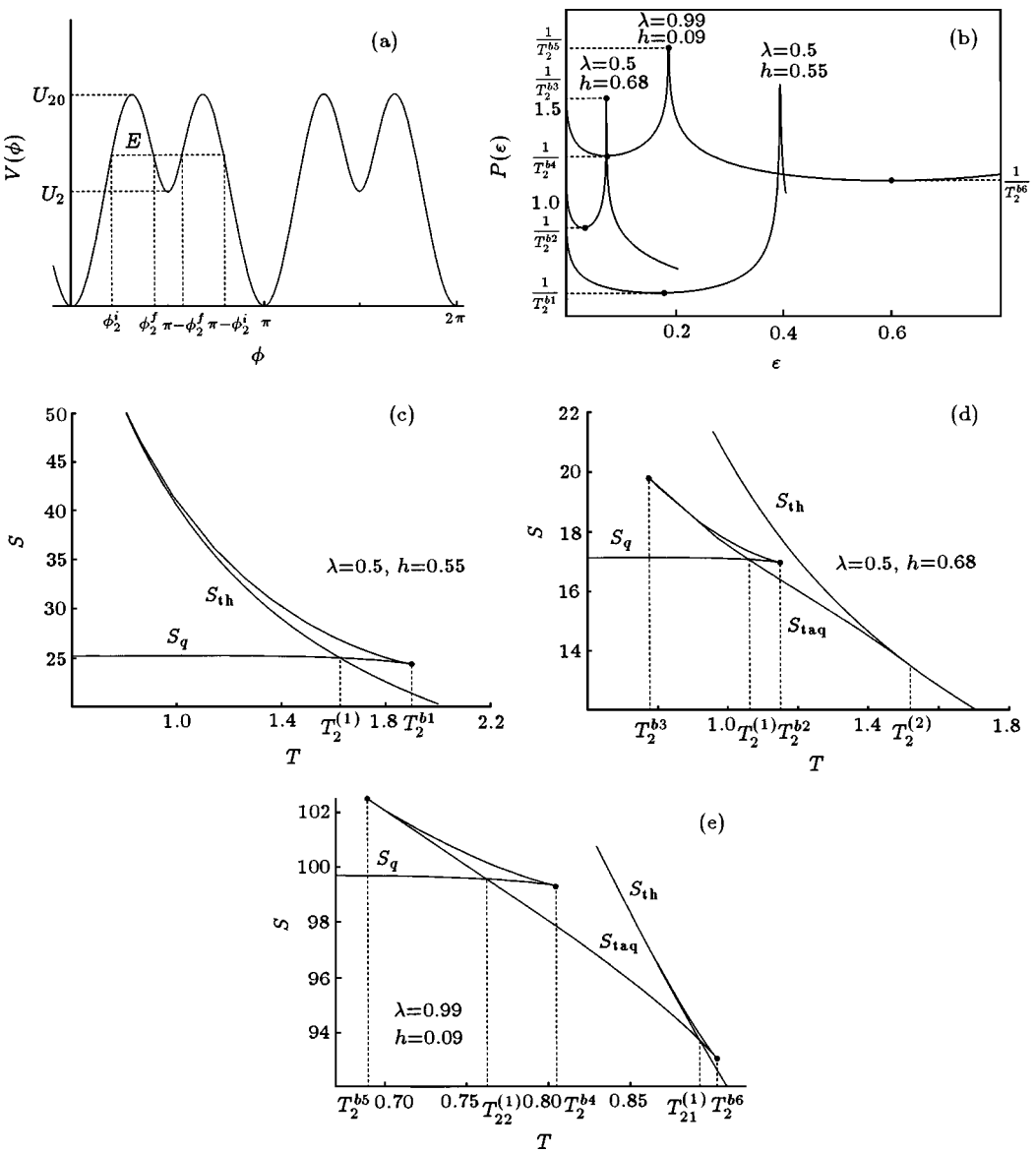


Fig.2. Potential, periods of periodic instantons and action-temperature diagrams for $\lambda = 0.5$, 0.99 and $1 - \lambda < h < \sqrt{1-\lambda}$ with $S^2 = 100$ and $K_2 = 1$. (a) Effective potential. (b) The periods of periodic instantons. (c) Type II: first-order transition (one bifurcation point). (d) Type III: the second-order transition followed by a first-order transition (two bifurcation points). (e) Type IV: the first-order transition followed by another first-order transition (three bifurcation points).

3.3. The case of $(1-\lambda)^{1/2} < h < 1$

When $\sqrt{1-\lambda} < h < 1$, $\phi = 0$ and $\phi = \pi$ are still two degenerate states, though the minima at $\phi = \pm\frac{\pi}{2}$ become the global minima. For the trajectory with energy E such that $0 < E < U_{30}$ ($U_{30} = U_{20}$) the period of periodic instanton and Euclidean action have the same forms as Eq.(18) and Eq.(19). In the case only type I of transition occurs in the crossover from the quantum to the classical regime.

4. Conclusion

We have studied the crossover of the quantum-classical transition of the escape rate of a biaxial ferromagnet with a magnetic field applied along the hard anisotropy axis. We show that the type of transition can be determined by counting the number of bifurcation points in the action-temperature diagram, in agreement with theoretical prediction in Refs.[16,1]. The type of phase transition depends on the values of the parameters λ and h which determine the shape of the effective potential. Since the magnetic field applied along hard axis can control the shape of the effective potential for given λ, besides the known type I and II of transition, the type III and IV of transition occur in the region of appropriate values of the parameters λ and h. This indicates that it is important to vary the shape of potential by adjusting environmental parameters in order to observe rich quantum tunnelling phenomena.

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