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Transition Phase Diagram for Escape Rate of Nanospin System in an Applied Magnetic Field

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We have investigated the escape rate of nano-magnetic particle with a magnetic field applied along the easy axis. The model studied here is described by the Hamiltonian $H = K_1 \hat{S}_z^2 + K_2 \hat{S}_y^2 + g\mu_b B\ \hat{S}_x\ (K_1 > K_2 > 0)$ and the escape rate was calculated with in the semiclassical approximation. We have obtained a diagram for orders of the phase transition depending on the anisotropy constant and the external field. For $K_2/K_1 > 0.85$ the present model reveals the existence of the first order transition within the quantum regime.

Key words : escape rate, quantum tunneling, phase diagram, Euclidean potential

1. Introduction

In recent years there has been much interest in the problem of the magnetization reversal of a nanospin particles [1]. It is well known that there are two possible mechanisms of the magnetization reversal: a classical thermal activation [2] and a quantum tunneling [3-5]. In the study of this problem the transition rate of the system of magnetic particles is mainly concerned. At high temperature the transition rate is governed by classical thermal activation, but when the temperature is very low the quantum tunneling dominates. As the temperature is lowered the phase change of the transition rate between the classical thermal activation and the quantum tunneling occurs. This phase transition can be either first order [6] or second order [7]. In recent several works [8-10] it is shown to be possible in the real system such as single-domain ferromagnetic particle. The two types of phase transitions have been suggested by Chudnovsky [11]. However, the coexistence of the first order phase transition within quantum regime and the second order classical to quantum transition, which was also shown by Chudnovsky. In this paper we find an another system which shows all kinds of phase transition mentioned above.

Consider a nanospin particle with an applied field B along the easy axis. If the spin particle is a uniaxial spin system with XOY easy plane anisotropy and the easy X-axis in the XY-plane the Hamiltonian for this system is given by

$$H = K_1\ \hat{S}_z^2 + K_2\ \hat{S}_y^2 + g\mu_b B\ \hat{S}_x \tag{1}$$

where K_1 and K_2 are the anisotropy constants, μ_b is the Bohr magneton, and g is the spin g-factor which is taken to be 2.0 here. Since we choose XY-plane as the easy plane the anisotropy constants satisfies $K_1 > K_2 > 0$.

The anisotropy energy associated with this Hamiltonian has two local energy minima; the one on the X-axis which is metastable state and the other on the ($-X$) axis. Between these two energy minima there exists an energy barrier, and the spin escapes this metastable state either by crossing over or by tunneling through the barrier.

In the coherent spin state representation [12] the effective Lagrangian corresponding to the Hamiltonian, Eq. (1), for small deviation from the easy plane is written as

$$L(\phi,\dot{\phi}) = \dot{\phi}\hbar S_z - \langle \theta,\phi|H|\theta,\phi\rangle = \hbar^2\frac{m(\phi)}{2}\dot{\phi}^2 - V(\phi) \tag{2}$$

where

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

is an effective mass, and

$$V(\phi) = K_2S^2(\sin^2\phi + \alpha\cos\phi + \alpha) \tag{4}$$

is an effective potential for the spin system. Here we have introduced dimensionless parameters $\lambda = K_2/K_1 (< 1)$, $\alpha =$

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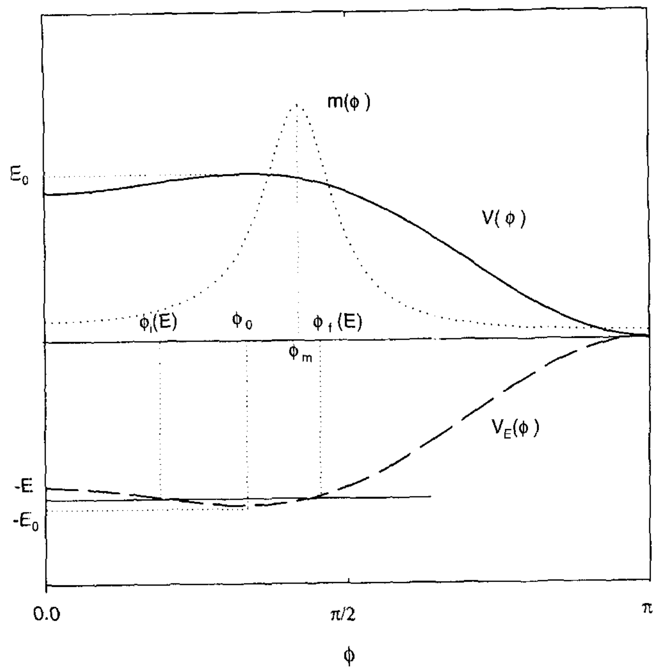

Fig. 1. The effective potential $V(\phi)$ (solid), Euclidean potential $V_E(\phi)$ (dashed), and the effective mass $m(\phi)$ (dotted). ϕ_0 is the position at which the Euclidean potential has a minimum, while ϕ_m the position at which the effective mass has a maximum. $\phi_i(E)$ and $\phi_f(E)$ are the classical turning points at Euclidean energy $-E$.

$2B/B_c(B_c=K_2S/\mu_b$ is coercive field), and added a constant term $K_2S^2\alpha$ in the effective potential for convenience. The effective mass and potential are shown in Fig. 1. The barrier height of $V(\phi)$ decrease as α should have values between 0 and 2. We note that the mass depends on ϕ. Later we will see that the ϕ dependence of the effective mass plays a crucial role for the occurrence of the first order phase transition in quantum regimes.

At temperature T the escape rate of spin can be obtained by taking ensemble average of the tunneling probability. Introducing Euclidean-time $\tau = it$ this can be written as the path integral form [13-15]

$$\Gamma(\tau)=\int d[\phi(\tau)]\, \exp\frac{1}{\hbar}\oint d\tau\left[\hbar^2\frac{m\dot{\phi}}{2}\dot{\phi} - V_E(\phi)\right], \tag{5}$$

where $V_E(\phi)=-V(\phi)$ is the Euclidean effective potential (see Fig. 1), and $\dot{\phi}\equiv d\phi/d\tau$. In the semi classical approximation, neglecting the quantum fluctuation term, the escape rate at an energy E above the metastable minimum is given by

$$\Gamma(\tau)\sim e^{-\frac{1}{\hbar}S(\tau)} \tag{6}$$

where $S(\tau)$ is the minimum effective Euclidean action which can be obtained by taking the smallest value of S_0 and $S(T)$. Here S_0 is thermodynamic action defined by

$$S_0=\frac{\hbar E_0}{k_BT} \tag{7}$$

with $E_0=\dfrac{K_2S^2}{k_BT}(\alpha+2)^2$, and $S(T)$ is expressed as

$$S(T)=2\hbar\int_{\phi_i(E)}^{\phi_f(E)} d\phi\sqrt{2m(\phi)[V(\phi)-E]}+\frac{\hbar E}{k_BT} \tag{8}$$

where $\phi_i(E)$ and $\phi_f(E)$ are the solution of the equation $V(\phi) = E$. For $E=2\alpha K_2S^2$ which is the bottom of the metastable state the Euler-Lagrange equation gives the bounce solution. When $2\alpha K_2S^2 < E < K_2S^2(\alpha+2)^2/4$ the trajectory $\phi(\tau)$ in $V_E(\phi)$ shows periodic motion with turning points at $\phi_i(E)$ and $\phi_f(E)$. The solution corresponding to this trajectory is called the periodic instanton whose period is defined as

$$\tau_p(E)\equiv\frac{\hbar}{k_BT}=\hbar\int_{\phi_i(E)}^{\phi_f(E)} d\phi\frac{\sqrt{2m(\phi)}}{V(\phi)-E} \tag{9}$$

We now examine how the period τ_p changes as a function of energy E. Since the effective mass depends on ϕ it influences on the variation of τ_p with E. To see this we look into the Eq. (3). For small values of λ, since $m(\phi)$ varies not much it gives little effect on the behavior of τ_p. However, as λ comes close to 1, the magnitude of the effective mass at turning points is small at first, then rises rapidly (see Fig. 1). As the mass becomes larger the speed of a particle in the potential $V_E(\phi)$ reduces, and it takes more time to complete the periodic motion in $V_E(\phi)$.

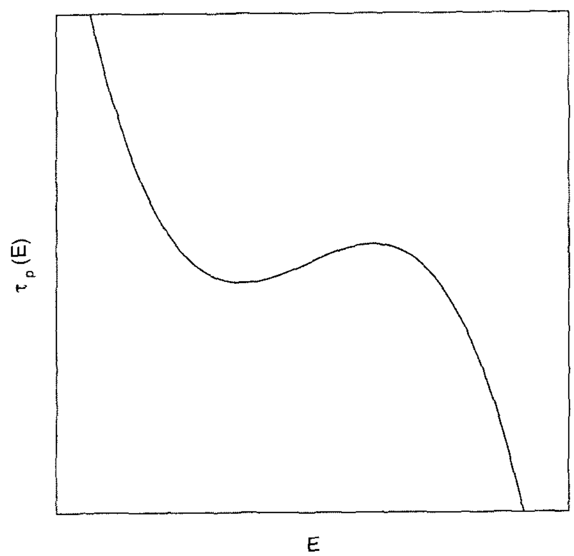

Fig. 2. The period in Euclidean potential as a function of energy at $\lambda = 0.9$ and $\alpha = 1.0$, which shows the first order phase transition within the quantum regime.

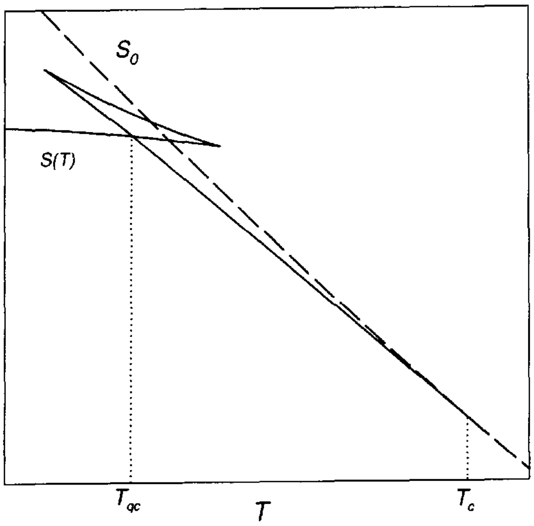

Fig. 3. The actions $S(T)$ and S_0 as a function of temperature at $\lambda = 0.9$ and $\alpha = 1$. T_c corresponds to classical to quantum crossover temperature and T_{qc} to the transition temperature between the different quantum regime.

Thus, the period τ_p decreases with E at the start, but then changes to increase due to the rapid increase of $m(\phi_f)$. We now note that the maximum point of the effective mass ϕ_m does not coincide with the minimum point of the Euclidean potential ϕ_0, which is illustrated in Fig. 1. Therefore, as E approaches to the top of the potential barrier the motion of the particle in $V_E(\phi)$ is restricted in a region where the effective mass becomes small. Thus, in this region, τ_p decreases with E. This suggests that the whole behavior of τ_p will be the form illustrated in Fig. 2. As proposed in Ref. [11] this form produces the first order phase transition inside the quantum tunneling region.

In Fig. 3 we have plotted the effective action as a function of T for $\alpha = 1$ and $\lambda = 0.9$. At $T = T_c$ the escape rate changes from the thermal activation to the quantum tunneling regime, and the transition is second order. Below T_c as T is lowered, the minimum action increases smoothly at first, changes abruptly at T_{qc} (the cusp an $T = T_{qc}$ in the figure), and then becomes almost constant. The quantum regime is thus, divided into two parts: the thermally assisted quantum tunneling ($T_{qc} < T < T_c$) and the pure quantum tunneling ($T < T_{qc}$). It can be seen from this picture that the phase transition at $T = T_{qc}$ is first order.

According to our numerical calculations that orders of the phase transitions are relevant to both α and λ. In Fig. 4. we have drawn a diagram for the orders of the phase transitions in (λ, α) plane. As remarked earlier the maximum value of α is 2 in the spin system. However, since we are interested in the positive effective mass α is

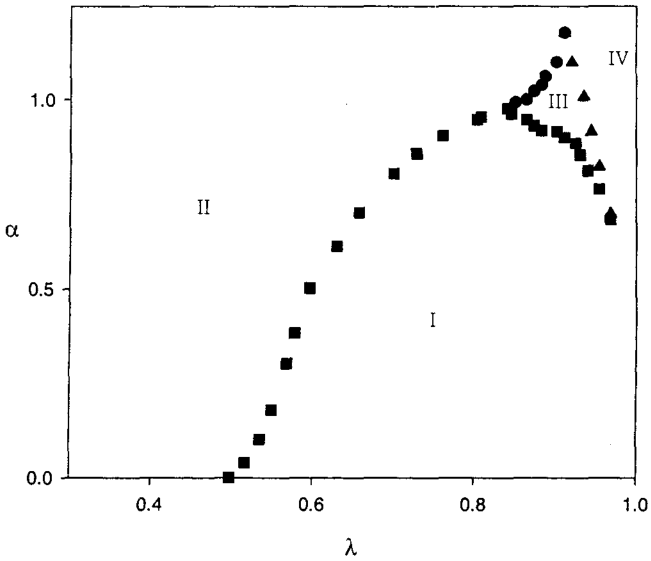

Fig. 4. The phase diagram for the orders of phase transition in (λ, α) plane. Region I: the first order classical to quantum transition. Region II: the second order classical to quantum transition. Region III: the second order classical to quantum transition and the first order transition with in quantum regime coexist. Region IV: the negative effective mass area.

restricted by inequality

$$\lambda\left(1 + \frac{\alpha^2}{16}\right) < 1 \qquad (10)$$

From the diagram we observe many interesting result. First, the classical to quantum phase transition shows both the first order (region I) and the second order (region II) transitions. Note that there is only the second-order transition for $\lambda < 0.5$. For materials with λ larger than 0.5 we can see that the order changes from first to second as α increases, and the phase boundary increases with λ up to 0.85, after which it decreases.

In the case of the phase transition within the quantum regime there is no phase transition for λ below 0.85. However, for $\lambda > 0.85$, there exists phase transition which is first order. We also observe that for $0.85 < \lambda < 0.91$ the phase boundary starts from the value corresponding to the maximum of the phase boundary between regions I and II and increases with λ. When λ becomes larger than 0.91, however, the phase boundary decreases with λ due to the positive mass condition, Eq. (9). This phase boundary forms a new region III where both the first order transition within the quantum regime and the second order classical to quantum transition coexist. Finally, in the region IV, since the negative effective mass begins to appear the phase transition cannot be defined.

Our speculation about these results is as following. For materials with small λ the height of the potential barrier is small. In an ensemble of nanospin particles each will then be relaxed to reverse its magnetization easily, which leads to the smooth variation of the escape rate with temperature T. On the other hand, if λ is large the barrier height will become large, and hence the spin particle will be reluctant to reverse its magnetization. In this case it needs the energy such as latent heat to make the spin particles ready to reverse their magnetization. Therefore, the escape rate experiences the first order phase transition.

We can also discuss the change of the order with α for a given λ. For less than 0.5, since the barrier height is essentially small for all values of α, the nanospin particle can easily reverse its magnetization, which corresponds to the second order transition. For $0.5 < \lambda < 0.85$, the barrier height is large at small α, but it becomes smaller as α increases. It is possible for the order to change from first to second with increasing α. We now consider the case $\lambda > 0.85$. When α is small the barrier height is so large that only the high temperature first order transition occurs at lower temperature, i.e., quantum region, with the classical-to quantum transition being changed in to second order. This leads to the first order transition in quantum tunneling region. As α further increases, the external field makes the magnetization reversal easy (small barrier height), the situation is same as the case of small λ.

In conclusion, we have investigated the phase transition for the escape rate from metastable states in nanospin system with a magnetic field applied along the easy axis. We found the coexistence of the first order phase transition within the quantum tunneling region and second order classical to quantum transition for large λ and α. Futhermore, the phase diagram for the orders of the phase transitions in (λ, α) plane is obtained.

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