Study Phase Transition Properties of a Ferroelectric Nanoparticle with the Usual Mean-Field Approximation

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Abstract—By using the usual mean-field approximation, the phase transition properties of a ferroelectric nanoparticle described by the transverse field Ising model have been studied. The exchange interactions and transverse fields at the surface are assumed to be different from those of the interactions parameters in the bulk. The phase diagrams for the ferroelectric nanoparticle with a size S are calculated in the (Tc, Js) coordinates and the (Tc, Ωs) coordinates by two types of parameter modifications. In addition, the crossover features for interactions parameters of the ferroelectric nanoparticle are also examined.

Keywords-ferroelectric nanoparticle; transverse Ising model; phase diagram; Curie temperature

I. INTRODUCTION

In recent decades, the nano-materials have been paid attention more and more in experiment and theory [1-11]. In the experiment, it has been demonstrated that the magnetic properties of nanoparticle-based systems are deviated from the corresponding bulk nano-materials [1]. As we all know, these magnetic features can be easily changed due to the finite-size effects or surface effects while the particle size decreases. The study of nanoparticle magnetism seems to be one of the current topics in magnetism. In the theory, the transverse field Ising model has been thought to be a good candidate to describe the phase transitions in the ferroelectric nano-systems. The effective-field theory with correlations and the usual mean-field approximation have been used to inspect various physical properties of the ferroelectric nano-systems [3-11]. Kaneyoshi has studied the phase diagrams of a ferroelectric nanoparticle by changing the particle size S as well as two ratios of s and p for the exchange interactions and the transverse fields between the corresponding value at the surface and the corresponding value in the bulk within the two frameworks of the effective-field theory with correlations and the usual mean-field approximation. The results indicate that the critical behaviors of interaction parameters are a little different from those of the ferroelectric thin films [3]. Afterwards, Kaneyoshi also calculated the thermal variations of the longitudinal and transverse magnetizations in the ferroelectric nanoparticle by the use of the usual mean-field approximation [4]. Recently, Kaneyoshi [5, 6] discussed the phase diagrams

and magnetizations in the ferroelectric nanoparticles with different structures with the effective-field theory with correlations. Very recently, Lu [7] investigated the dependence of the phase diagrams on the exchange interactions and transverse fields of a ferroelectric nanoparticle in the (T_c, J_s) coordinates and the (T_c, Ω_s) coordinates with the effective-field theory with correlations, however, this work has not been carried out by using the mean-field approximation up to now.

In this present paper, we will study the dependence of phase diagrams on exchange interactions and transverse fields for a ferroelectric nanoparticle in the (T_c, J_s) coordinates and the (T_c, Ω_s) coordinates. The numerical results are compared with the corresponding results of the effective-field theory with correlations. Meanwhile, the crossover features for interactions parameters are also calculated.

II. THE MODEL AND FORMULATIONS

The ferroelectric nanoparticle with a certain size S is assumed to be consisted of a two-dimensional arrangement of pseudo-spins, where the values of each pseudo-spin variable are $\sigma_{iz}=\pm1$. Figure 1 shows the schematic illustration for the ferroelectric nanoparticle with a different size S. It can be found that the ferroelectric particle is consisted of the concentric hexagonal rings. The pseudo-spins on a ring K ($0<K\leq S$) are on a same sublattice K. The pseudo-spins are connected to the nearest-neighbor pseudo-spins each other with spin exchange interaction. The Hamiltonian is [3, 4, 7]

$$H = -\sum_{ij} J_{ij}\sigma_{iz}\sigma_{jz} - \Omega_s \sum_{i\in s}\sigma_{ix} - \Omega_b \sum_{i\in b}\sigma_{ix}, \quad (1)$$

where σ_{iz} and σ_{ix} are the pseudo-spin operators. J_{ij} is the exchange interaction between the nearest-neighbor pseudo-spins at sites i and j. $J_{ij}=J_s$ or $J_{ij}=J_b$ represents both pseudo-spins are at the surface ring or the others. $\Omega_{ij}=\Omega_s$ or $\Omega_{ij}=\Omega_b$ denotes the transverse fields when pseudo-spins are on the surface rings or in the bulk rings.

Under the usual mean-field approximation, the longitudinal magnetizations in the z-direction of the ferroelectric nanoparticle with $S=2$ are given as follows [3]

$$m_1 = F_b(6J_b m_2) \quad \text{φορ K=1}, \quad (2)$$

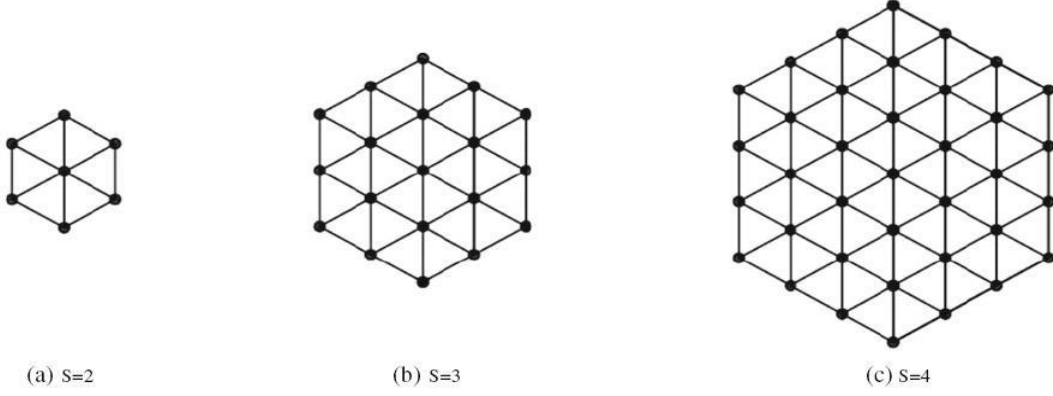$$m_2 = F_s(2J_s m_2 + J_b m_1) \quad \text{φορ K=2}, \quad (3)$$

Figure 1. Schematic illustration of a ferroelectric nanoparticle with a size S.

where the functions $F_b(x)$ and $F_s(x)$ are defined as

$$F_b(x) = \frac{x}{y_b}\tanh(\beta y_b) \quad , \tag{4}$$

with

$$y_b = \sqrt{x^2 + \Omega_b^2} \quad , \tag{5}$$

and

$$F_s(x) = \frac{x}{y_s}\tanh(\beta y_s) \quad , \tag{6}$$

with

$$y_s = \sqrt{x^2 + \Omega_s^2} \quad , \tag{7}$$

$\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the absolute temperature.

Similar to the ferroelectric nanoparticle with $S=2$, the longitudinal magnetizations for the ferroelectric nanoparticle with $S=3$ can also be obtained [3]

$$m_1 = F_b(6J_b m_2) \quad \text{φορ } K=1, \tag{8}$$

$$m_2 = F_b(2J_b m_2 + J_b m_1 + J_b m_{30} + 2J_b m_{31}) \quad \text{φορ } K=2, \tag{9}$$

and

$$m_{30} = F_s(2J_s m_{31} + J_b m_2) \quad \text{φορ } K=3, \tag{10}$$

$$m_{31} = F_s(2J_s m_{30} + 2J_b m_2) \quad \text{φορ } K=3. \tag{11}$$

Thus, the coupled equations of magnetizations for the ferroelectric nanoparticle with a certain size S can be easily derived with the framework of the mean-field approximation.

The right sides of the coupled equations for the ferroelectric nanoparticle with a certain size S can be expanded. As a result, we can neglect the nonlinear terms and only take into account the linear terms. Thus, the transition temperature T_c can be derived as the functions of J_s, J_b, Ω_s and Ω_b. The general equations for the two systems with $S=2$ and $S=3$ are obtained [3]:

$$1 = 6AB_1 + 2B_2 \quad \text{φορ } \Sigma=2, \tag{12}$$

$$[1 - 2A(1+3A)][1 - 4B_2^2] = AB_1(5+8B_2) \quad \text{φορ } \Sigma=3, \tag{13}$$

with

$$A = JF'(0), \quad B_1 = JF_s'(0), \quad B_2 = J_s F_s'(0). \tag{14}$$

Τηε χοεφφιχιεντσ A, B1, B2 αρε

$$A = \sinh(J_b\nabla)\cosh^5(J_b\nabla)F_b(x)|_{x=0}, \tag{15}$$

$$B_1 = \sinh(J_b\nabla)\cosh^2(J_s\nabla)F_s(x)|_{x=0}, \tag{16}$$

$$B_2 = \sinh(J_s\nabla)\cosh(J_s\nabla)\cosh(J_b\nabla)F_s(x)|_{x=0}. \tag{17}$$

where $\nabla = \partial/\partial x$ is the differential operator and $e^{\alpha\nabla}f(x) = f(x+\alpha)$.

III. NUMERICAL RESULTS

In this section, we will dicuss the phase transition properties of a ferroelectric nanoparticle with a certain size S from the general equations [12,13]. Usually, the phase diagram can be described by two ways: the relationships between the surface exchange interaction J_s and the Curie temperature T_c as well as the relationships between the
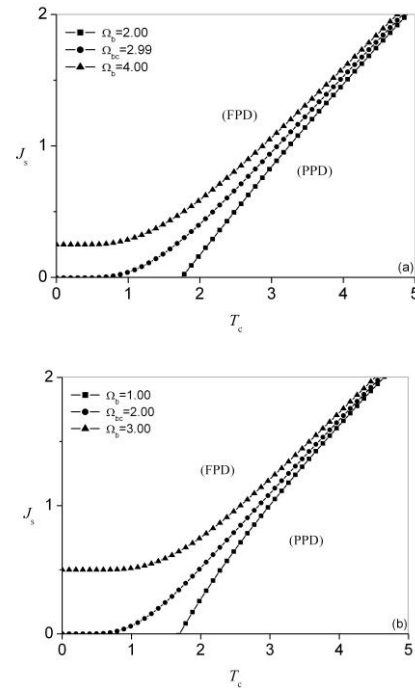

Figure 2. The dependence of the phase diagram on the bulk transverse field Ω_b. J_b=1.00, S=2. (a) Ω_s =2.00, (b) Ω_s=3.00.

surface transverse field Ω_s and the Curie temperature T_c, namely the curves of $J_s \sim T_c$ or $\Omega_s \sim T_c$. For simplicity and without loss of generality, we consider the ferroelectric nanoparticle with a particle size S changing from 2 to 5.

Figure 2 shows the dependence of the phase diagram on the bulk transverse field Ω_b, namely the curves of $J_s \sim T_c$ for different Ω_b. For a certain size S, it is obvious that the curve of $J_s \sim T_c$ depends sensitively on the bulk transverse field Ω_b. With the surface exchange interaction J_s increases, the Curie temperature T_c also increases monotonously. The smaller the bulk transverse field Ω_b, the larger the range of the ferroelectric phase region. The larger the bulk transverse field Ω_b, the larger the range of the paraelectric phase region. Thus, the phase diagram will be the ferroelectric-dominant phase diagram (FPD) or the paraelectric-dominant phase diagram (PPD). The FPD
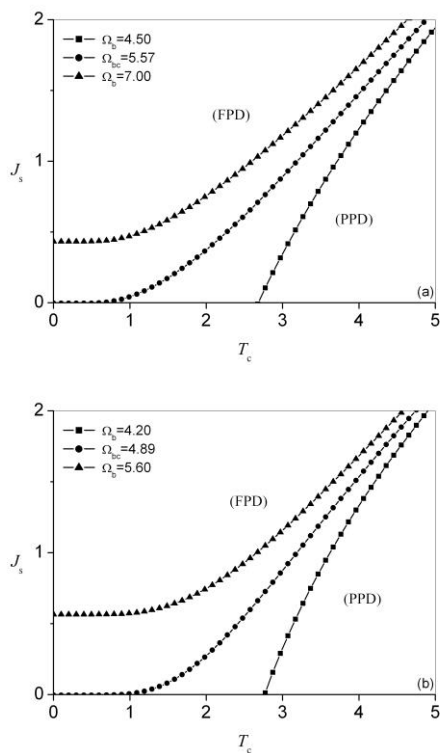
denotes that the phase diagram is only in a ferroelectric phase state when the temperature is below a certain value without respect to the surface exchange interaction J_s. That is to say, any J_s can result in a transition from the ferroelectric phase state to paraelectric phase state as the temperature increases. On the other hand, the PPD represents that the system is only in a paraelectric phase state when the surface exchange interaction J_s is below a certain value without respect to the temperature. In other words, only a larger J_s can result in a transition from ferroelectric phase state to paraelectric phase state as the temperature increases. Therefore, there exists a crossover value of the bulk transverse field Ω_b while the phase diagram changes from the FPD state to PPD state. It is obvious that the crossover value Ω_{bc} can also be obtained when the values of J_s and T_c reduce to zero at the same

Figure 3. The dependence of the phase diagram on the bulk transverse field Ω_b. J_b=1.00, S=3. (a) Ω_s =2.00, (b) Ω_s=3.00.
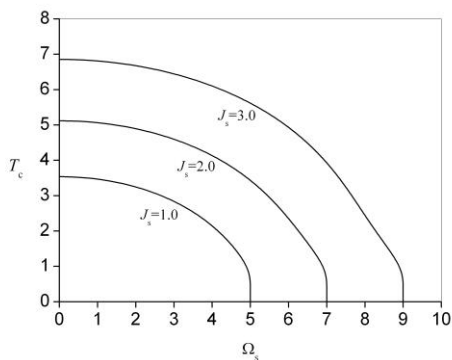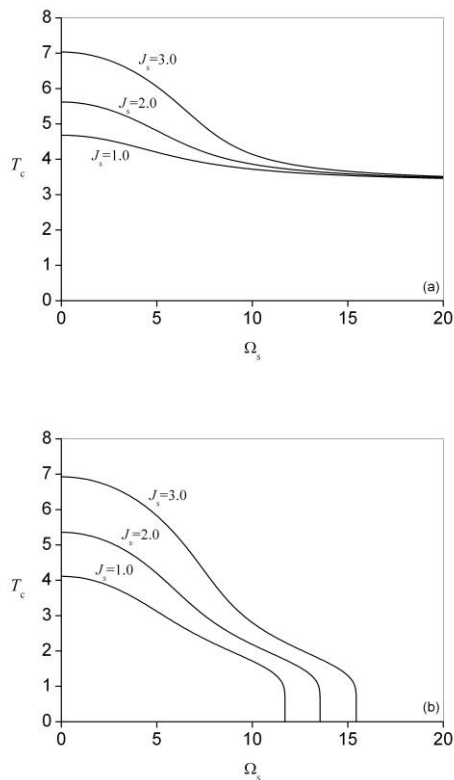

Figure 5. The dependence of the phase diagram on the surface exchange interaction J_S. J_b=1.00, S=3. (a) Ω_b=2.00, (b) Ω_b=4.00.

Figure 4. The dependence of the phase diagram on the surface exchange interaction J_S. J_b=1.00, Ω_b=2.00, S=2.
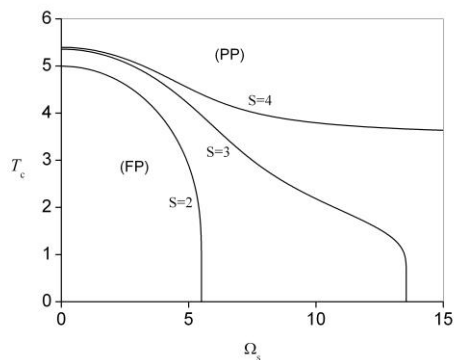

Figure 6. The dependence of the phase diagram on the ferroelectric nanoparticle size S. J_S=2.00, J_b=1.00, Ω_b=4.00.

time. Meanwhile, the effect of the surface transverse field Ω_s on the crossover value is also exhibited in Figure 2. The larger the surface transverse field Ω_s, the smaller the crossover value Ω_{bc}. Figure 3 is the same as Figure 2 but for a different particle size S. Obviously, the larger the particle size S, the larger the crossover value Ω_{bc}. These features in Figure 2 and 3 are similar to the corresponding result of the effective-field theory with correlations [5, 7].

Figure 4 shows the dependence of the phase diagram on the surface exchange interaction J_s, i.e., the curves of $T_c \sim \Omega_s$ for different values of J_s. For a certain J_s, with the surface transverse field Ω_s increases, the Curie temperature T_c decreases monotonously. Finally, the Curie temperature T_c will reduce to zero at a critical value of the surface transverse field Ω_s. Meanwhile, the effect of the surface exchange interaction J_s on the curves of $T_c \sim \Omega_s$ can also be found in Figure 4. For a certain surface transverse field Ω_s, the larger the surface exchange interaction J_s, the larger the Curie temperature T_c. Furthermore, there is a critical value of the Curie temperature T_c when the surface transverse field Ω_s reduces to zero.

Figure 5(a) is the same as Figure 4, but for a different particle size $S=3$. Now, it is obvious that the curves of $T_c \sim \Omega_s$ for different values of J_s will intersect at a common point as the increase of surface transverse field Ω_s. However, the curves of $T_c \sim \Omega_s$ will not intersect with the coordinate axis in x direction irrespective of the value of surface transverse field Ω_s. Figure 5(b) is the same as (a) but for a larger bulk transverse field Ω_b. Obviously, it is different from Figure 5(a), namely the curves of $T_c \sim \Omega_s$ for three different values of J_s intersect with the coordinate axis in x direction. It indicates that the curves of $T_c \sim \Omega_s$ for different values of J_s depends sensitively on the bulk transverse field Ω_b.

Figure 6 shows the dependence of the phase diagram on the size S of the ferroelectric nanoparticle. It can be seen from Figure 6, the curves of $T_c \sim \Omega_s$ are plotted as the function of S. The two curves for $S=2$ and 3 intersect with the x coordinate axis at a critical value of Ω_s, but the curve for $S=4$ does not intersect with the x coordinate axis. These features are also similar to the corresponding result of the effective-field theory with correlations [5, 7].

IV. CONCLUSION

In conclusion, the phase transition properties of a ferroelectric nanoparticle described by the transverse field Ising model have been studied by the usual mean-field approximation. By modifying exchange interactions and transverse fields at the surface, the phase diagrams in the (T_c, J_s) coordinates and the (T_c, Ω_s) coordinates are systematically discussed. It indicates that the results of the usual mean-field approximation are consisted with those of the effective-field theory with correlations.

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