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# Frustration in a transverse Ising nanoisland with an antiferromagnetic spin configuration

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ABSTRACT

The phase diagrams, saturation magnetizations and temperature dependences of magnetizations in a transverse Ising nanoisland with an antiferromagnetic spin configuration are studied by the uses of the effective-field theory with correlations (EFT) and the mean-field approximation (MFA), in order to clarify whether the MFA can be successfully applied to the theoretical discussions of naonoislands. From these investigations, we have found a lot of unexpected characteristic phenomena in these properties, when the value of an interlayer coupling takes a large value. We have also found that the applications of the MFA to the magnetic properties are extremely restricted for nanoislands, when the value of an interlayer coupling takes a large value, in contrast to a number of bulk studies.



## 1. Introduction

Nowadays, nanoscaled materials provide a rich variety of novel scientific knowledge and potentials for technological applications. In particular, much attention has been devoted experimentally and theoretically on clarifying the magnetic properties in nanoscaled magnetic materials, such as ultra-thin films, nanoparticles (including nanoislands), nanowires, nanotubes and so on. In these nanosystems, surface effects particularly give the distinct contributions to the magnetic properties, since a large fraction of the atoms in them exist at the surface They become more important when reducing the size of the materials. A lot of investigations indicate that the size reduction of a material down to a nanoscale gives the magnetic properties different from those in the bulk counterpart.

In a bulk magnetic material, the theoretical first step for the interpretation of magnetic properties has been normally the application of the mean-field approximation (MFA). The MFA has well explained the major aspects of the phenomena in a magnetic material, when used correctly [1]. It is also well-known that the MFA is not well-applied for the particular situations, especially for the examinations in the vicinity of critical temperature in a magnetic material and in the vicinity of critical concentration in a site–(or bond-) diluted magnetic material. The reason comes from the fact that the concept of the MFA is in considering only one atom and replaces the interactions from other atoms with a uniform field proportional to the averaged magnetization. In a nanoscaled system, on the other hand, the concept of core–shell has been successfully applied to the explanations of physical properties. Even when the core–shell concept is used, it is not clear whether the basic concept of the MFA can be successfully applied to the theoretical discussions of a nanoscaled magnetic system, since the magnetization at each site is heavily dependent on the surrounding situation in it. In fact, as has been discussed in [2,3], an interesting phenomenon, namely the reentrant phenomenon, has been found in many nanosystems described by the transverse Ising model (TIM), where the transverse field at the surface shell is taken by zero and the phenomenon has been induced by changing the value of transverse field in the core. But, one should notice that the reentrant phenomenon has not been obtained from the usage of the MFA, but also it has been found when the effective-field theory with correlations (EFT) [4,5] has been applied to them. The EFT corresponds to the Zernike approximation [6] and it is believed to give more exact results than those of the MFA, since it includes automatically some correlations between a central spin and the near neighbor spins. Except the above-mentioned situation (or the reentrant phenomenon), the MFA and the EFT have given the results similar to each other for the magnetic properties in the nanosystems [2,3]. The recent works for nanosystems [7,8] prove that the results obtained from the EFT have the same topology as those obtained from the MC(Monte Carlo simulation), while the results obtained from the MC are smaller than those of the EFT.

The TIM is generally believed to describe the phase transition of order–disorder type ferroelectrics. Because the TIM cannot be

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solved exactly, many approximations have been used to study the magnetic properties of various materials, such as the MFA and the EFT. In a series of recent works [9–11], the TIM has also been applied successfully to the investigations of nanoislands. The possibility of reentrant phenomena in these systems has been discussed within the theoretical framework of the EFT. In these works, however, we have not discussed whether the MFA can be successfully applied to the theoretical discussions of naonoislands, since the TIM nanoislands have exhibited the reentrant phenomenon free from disorder induced frustration. Traditionally, the reentrant phenomena have been found in a variety of disordered magnetic systems experimentally and theoretically [12,13], especially spin glass systems in which the effects of frustration due to the change of sign in exchange interactions play important ingredient. A ferromagnet in a random field also exhibits the reentrant phenomena, which is equivalent to the Ising antiferromagnet with randomly quenched exchange interactions in a uniform field [14]. Furthermore, the magnetic properties of a TIM nanoisland with an antiferromagnetic spin configuration has not been examined by the use of the EFT and the MFA.

The aim of this work is, within the two theoretical frameworks of the MFA and the EFT, to investigate whether the MFA can be successfully applied to the theoretical discussions of the TIM naonoislands with an antiferromagnetic spin configuration and a ferromagnetic spin configuration, since, as discussed in [9–11], the TIM nanoislands may exhibit the reentrant phenomenon free from disorder induced frustration. In Section 2, the models and formulations for the nanoisland with an antiferromagnetic spin configuration are given by the use of both the EFT and the MFA, since the formulation based on the EFT for the same nanoisland with a ferromagnetic spin configuration have been discussed in the previous work [9]. In Section 3, the phase diagram, the saturation magnetization at $T=0.0$ K and the thermal variations of magnetizations in the two TIM naoislands are reported by the use of both the MFA and the EFT. From these examinations, we have found a lot of unexpected characteristic phenomena in these magnetic properties. Furthermore, we have found that the applications of the MFA to the magnetic properties are extremely restricted for the nanoislands, when the value of an interlayer coupling takes a large value, in contrast to a number of bulk studies. In Section 4, the thermal variations of magnetizations are examined in detail. Some unexpected behaviors have been found for them. Section 5 includes the conclusions.

## 2. Models and formulation

We consider the three-dimensional nanoisland (or particle) with an antiferromagnetic spin configuration, as depicted in Fig. 1. Each site on the figure is occupied by an Ising spin. The spins (or black and white circles) on the surface shell are coupled to the center (core) spin (or balck circle) with an exchange interaction $-J$ ($J>0.0$). The atoms on the surface shell are connected by the exchange interaction $-J_S$. The black and white circles represent the magnetic atoms with the up-spin and the down-spin directions, respectively. Each spin on the upper layer is connected to the corresponding magnetic atoms on the lower layer with an exchange interaction $J_R$ ($J_R>0.0$). As noted in [9–11], these choices come from the experimental facts [15–17].

The Hamiltonian of the system is given by

$$H = J_s \sum_{(ij)} \sigma_i^Z \sigma_j^Z + J \sum_{(mn)} \sigma_m^Z \sigma_n^Z - J_R \sum_{(im)} \sigma_i^Z \sigma_m^Z - \Omega s \sum_{(i)} \sigma_i^X - \Omega \sum_{(m)} \sigma_m^X \quad (1)$$

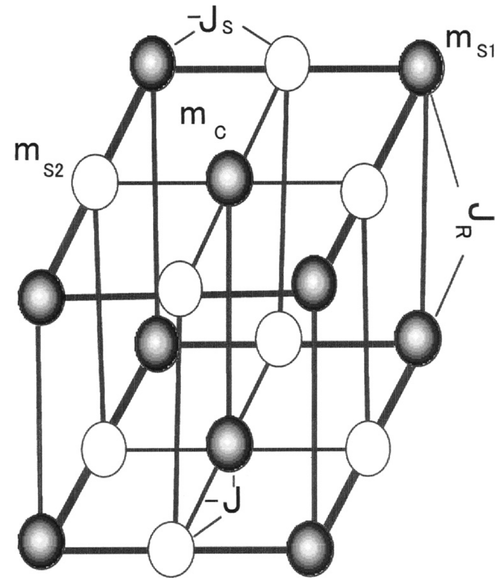


**Fig. 1.** Schematic representations of a nanoisland with an antiferromagnetic spin configuration. The black circles represent spin-1/2 magnetic atoms with the up-spin direction. The white circles are spin-1/2 magnetic atoms with the down-spin direction. The lines connecting the white and black circles represent the nearest-neighbor exchange interactions ($-J_S$, $J_R$ and $-J$).

where $\sigma_i^\alpha$ ($\alpha=z, x$) is the Pauli spin operator with $\sigma_i^Z = \pm 1$. $\Omega_S$ and $\Omega$ represent the transverse fields at the surface shell and in the core, respectively. The first ($ij$) term in the Hamiltonian (1) represents the contribution from the surface shell and the second ($mn$) term shows the interaction between the central atom and the atom on the surface shell. The third term is the contribution from the interlayer interaction. The surface exchange interaction $J_S$ is often defined as

$$J_S = J(1 + \Delta_S) \quad (2)$$

in order to clarify the effects of surface on the physical properties in the system.

For the system shown in Fig. 1, there exist two longitudinal magnetizations ($m_{S1} = <\sigma_i^Z>$ and $m_{S2} = <\sigma_j^Z>$) on the surface shell and a longitudinal magnetization ($m_C = <\sigma_m^Z>$) on the core in the $z$ direction. By the use of the MFA and the EFT, we can easily obtain the two longitudinal magnetizations at the surface shell and the longitudinal magnetization in the center as coupled equations, namely for the MFA,

$$m_{S!} = F_S\left(-2J_S m_{S2} + J_R m_{S1}\right)$$
$$m_{S2} = F_S\left(-2J_S m_{S1} - Jm_C + J_R m_{S2}\right) \quad \text{and}$$
$$m_C = F\left(-4Jm_{S2} + J_R m_C\right) \quad (3)$$

Here, the functions $F_S(x)$ and $F(x)$ are defined by

$$F_S(x) = \left(x/y_S\right)\tanh(\beta y_S) \quad \text{and}$$
$$F(x) = (x/y)\tanh(\beta y) \quad (4)$$

with

$$y_S = (x^2 + \Omega_S^2)^{1/2}$$
and
$$y = (x^2 + \Omega^2)^{1/2} \quad (5)$$

where $\beta = 1/k_B T$ and $T$ is a temperature. Within the EFT [4,5], they are given by