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Spatial Distribution of Magnetization in the Pyramid-Like Ising Nanoscopic System Interacting with the Substrate

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We study thermodynamic properties of an Ising model of a ferromagnetic nanoscopic pyramid deposited onto a ferromagnetic bulk substrate. The influence of the interaction between the pyramid and the substrateis calculated in terms of the reduced-state (density) operator used for description of thermodynamic properties of nanoscopic systems. The spatial distribution of the magnetization in the nanoscopic pyramid is obtained in the molecular field approximation.

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1. Introduction

During the past two decades we have witnessed significant advances in the ability to synthesize nanoscale structures as well as development of novel experimental method allowing exploration of their physical properties. This is exciting for two reasons. Firstly, new forms of matter with no counterpart in nature and revealing unique physical properties have been fabricated. Secondly, we have now realized nanostructures that open new avenues for development of very small devices.

Nanoscopic magnetic systems have always been very attractive from the theoretical point of view. On the other hand, studies of nanoscopic systems are characterized by a close coupling between theory and experiment because of rapidly increasing number of experimental works on real nanoscopic materials [1]. These materials often correspond remarkably close to certain idealized spin models and are great challenges not only for physicists, but also for chemists and engineers.

In experiments aiming at the investigation of nanoscopic systems we deal frequently with such systems deposited on a bulk substrate. However, most often in the theoretical description of such experiments the interaction between the nanosystem and the substrate is neglected. The main purpose of this work is to

find a way to include this and calculate its effect on the thermodynamic properties of the Ising model of a ferromagnetic nanoscopic system. To achieve this we apply the reduced-state (density) operator [2,3] and carry out the calculations within the molecular field approximation (MFA).

2. The model

It was shown recently that nanoscopic structures in the form of pyramids or similar shapes can be fabricated on a bulk substrate [4, 5].

In this paper we consider only magnetic properties of a nanoscopic pyramid. They are well described by the simple model of localized and ordered spins with the following spin-1/2 Hamiltonian

$$H = -\tfrac{1}{2} I \sum S^z_{\boldsymbol{f}l} S^z_{\boldsymbol{f}'l'}, \tag{1}$$

where I is the coupling parameter and $\sum$ stands for summation over pairs of different simple cubic (sc) lattice points. Our considerations are restricted to nearest-neighbor interaction only.

In Eq. (1) $\boldsymbol{f}$ denotes the two-dimensional position vectors of a spin belonging to a given monoatomic layer $l = 1, 2, 3, 4$ of the pyramid. There are 4 spins in the $l = 1$ layer, 16 spins in the $l = 2$ layer, 36 spins in the $l = 3$ layer, and 64 spins in the $l = 4$ layer. The total number of spins in the pyramid is 120 (see Fig. 1).

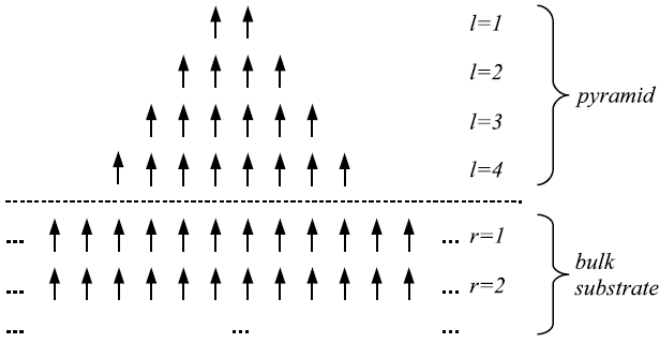

Fig. 1. Schematic diagram of ferromagnetic nanoscopic pyramid deposited on a ferromagnetic bulk substrate.

We assume that the nanoscopic pyramid is deposited on a bulk ferromagnetic substrate sufficiently well described by the spin-1/2 Ising model for a simple cubic lattice and the Hamiltonian

$$H_s = -\tfrac{1}{2} I_1 \sum S^z_{\boldsymbol{g}r} S^z_{\boldsymbol{g}'r'}. \tag{2}$$

Here $\boldsymbol{g}$ denotes the two-dimensional position vectors of spin belonging to a given monoatomic layer. The summations always run over different sites. The substrate is divided into monoatomic layers parallel to the planes (100) of a sc lattice. The position of each layer is given by the number $r = 1, 2, \ldots$

Let us assume that the interaction of the nanoscopic pyramid with the bulk substrate is described by the Heisenberg Hamiltonian of the form

$$H_I = -\tfrac{1}{2} I_2 \sum_{\boldsymbol{fg}} \boldsymbol{S}_{\boldsymbol{f}l=4} \boldsymbol{S}_{\boldsymbol{g}r=1}. \tag{3}$$

In order to take into account the interaction of the nanoscopic pyramid with the bulk substrate we shall apply the equilibrium reduced-state (density) operator [2, 3] suitable for description of a physical situation similar to the one we are concerned with. In deriving this reduced-state operator we use the fact that although the Universe as a whole is in the pure state, its arbitrary multiparticle parts are inevitably in mixed states. This is purely a quantum effect following from the holistic properties of the quantum theory, formally related to the fact that the Universe (according to the quantum cosmology postulates) has one vector of state common for all systems and, in the case of interactions among them, we are not able to specify the vector of state for individual subsystem (it may not be the case for the interactions of the effective field type or classical ones). Such a situation does not occur in the classical description because we may know classical trajectories of each particular molecule irrespective of their interactions. The holistic features of the quantum theory imply the use of the formalism of the reduced-state operators in description of multiparticle systems. For this reason the interaction (3) of the nanoscopic pyramid with the bulk substrate cannot be described by the Ising Hamiltonian.

In our case this reduced-state operator d takes the following form [2]:

$$d = \exp(\beta(F - H - H'(\beta))), \tag{4}$$

where F is the free energy and

$$H'(\beta) = \mathrm{Tr}_s\Big(H_I \exp(\beta(F_s - H_s))\Big) \tag{5}$$

is an effective term describing the interaction between the pyramid and the bulk substrate, $\mathrm{Tr}_s(\ldots)$ is the partial trace over the substrate states, $\beta = (k_{\mathrm{B}}T)^{-1}$, and

$$F_s = -\frac{1}{\beta} \ln \mathrm{Tr}_s\Big(\exp(-\beta H_s)\Big) \tag{6}$$

is the free energy of the substrate. Substituting expression (3) into Eq. (5) with the assumption that

$$|\langle S^x_{\boldsymbol{g}r}\rangle|, |\langle S^y_{\boldsymbol{g}r}\rangle| \ll |\langle S^z_{\boldsymbol{g}r}\rangle|, \qquad I_2 \ll I_1, \tag{7}$$

we arrive at

$$H'(\beta) = -\tfrac{1}{2} I_2 \langle S^z_{r=1}\rangle \sum_{\boldsymbol{f}} S^z_{\boldsymbol{f}l=4}, \tag{8}$$

where

$$\langle S^z_{r=1}\rangle = \mathrm{Tr}_s\Big(S^z_{\boldsymbol{g}r=1} \exp(\beta(F_s - H_s))\Big) \tag{9}$$

is the average bulk substrate spin moment in the layer $r = 1$.

3. Spatial distribution of magnetization

We describe the thermodynamic properties of the nanoscopic pyramid within the MFA. In order to achieve this we shall make use of the equilibrium reduced--state (density) operator (4). As a starting point of MFA we choose the following approximation of the operator(4):

$$d = \exp\Big(\beta(F - H - H'(\beta))\Big) = \exp\Big(\beta(F - H_0 - H_1 - H'(\beta))\Big)$$
$$\simeq d_0 = \exp\Big(\beta(F_0 - H_0 - H'(\beta))\Big), \tag{10}$$

where

$$F_0 = -\frac{1}{\beta}\ln \mathrm{Tr}\Big(\mathrm{e}^{-\beta(H_0+H'(\beta))}\Big), \tag{11}$$

$$H = (H - H_1) + H_1 = H_0 + H_1 \tag{12}$$

and the perturbative part H_1 of the Hamiltonian (1) is defined by the transformation

$$h \to H_1 = H(S^z_{\boldsymbol{f}l} \to \delta S^z_{\boldsymbol{f}l}), \tag{13}$$

$$\delta S^z_{\boldsymbol{f}l} = S^z_{\boldsymbol{f}l} - \langle S^z_{\boldsymbol{f}l}\rangle_0 \tag{14}$$

is the fluctuation operator of the z-component of the spin operator and

$$\langle S^z_{\boldsymbol{f}l}\rangle_0 = \mathrm{Tr}\Big(S^z_{\boldsymbol{f}l}d_0\Big) = \tfrac{1}{2}\hbar\tanh\Big(\tfrac{1}{2}\hbar\beta(I\sum_{\boldsymbol{f}'l'}\langle S^z_{\boldsymbol{f}'l'}\rangle_0 + I_2\delta_{l,4}\langle S^z_{r=1}\rangle_0)\Big). \tag{15}$$

Besides, H_0 is the Hamiltonian (1) in the molecular field approximation. Similarly, according to Eq. (9) the mean magnetization $\langle S^z_r\rangle$ of the bulk substrate in the MFA satisfies the equation

$$\langle S^z_r\rangle = \mathrm{Tr}_s\Big(S^z_r\exp(\beta(F_s - H_s))\Big) = \mathrm{Tr}_s\Big(S^z_r\exp(\beta(F_s - H_{s0} - H_{s1}))\Big) \simeq \langle S^z_r\rangle_0$$
$$= \mathrm{Tr}_s\Big(S^z_r\exp(\beta(F_{s0} - H_{s0}))\Big)$$
$$= \tfrac{1}{2}\hbar\tanh\Big(\tfrac{1}{2}\hbar\beta I_2\sum_{\boldsymbol{g}r'}\langle S^z_{r'}\rangle_0\Big), \tag{16}$$

where

$$H_s = (H_s - H_{s1}) + H_{s1} = H_{s0} + H_{s1}, \tag{17}$$

$$H_{s1} = H(S^z_{\boldsymbol{g}r} \to \delta S^z_{\boldsymbol{g}r}), \tag{18}$$

$$\delta S^z_{\boldsymbol{g}r} = S^z_{\boldsymbol{g}r} - \langle S^z_r\rangle_0, \tag{19}$$

$$F_{s0} = -\tfrac{1}{\beta}\ln \mathrm{Tr}_s\Big(\mathrm{e}^{-\beta H_{s0}}\Big) \tag{20}$$

and H_{s0} is the Hamiltonian substrate (2) in the MFA.

After introducing the following reduced magnitudes:

$$X_{\boldsymbol{f}l} = \frac{2}{\hbar}\langle S^z_{\boldsymbol{f}l}\rangle_0, \quad y_r = \frac{2}{\hbar}\langle S^z_r\rangle_0, \quad t = \frac{4k_{\mathrm{B}}T}{\hbar^2 I}, \quad a = \frac{I_2}{I}, \quad b = \frac{I_1}{I}, \tag{21}$$

Eqs. (15) and (16) can be written in the compact form

$$X_{\boldsymbol{f}l} = \tanh\Big(\frac{1}{t}\Big(\sum_{\boldsymbol{f}'l'} X_{\boldsymbol{f}'l'} + a\delta_{l,4}y_1\Big)\Big), \tag{22}$$

$$y_r = \tanh\Big(\frac{b}{t}\sum_{\boldsymbol{g}r'} y_{r'}\Big), \tag{23}$$

where

$$\delta_{l,4} = \begin{cases} 1 & \text{for} \quad l = 4, \\ 0 & \text{for} \quad l \neq 4. \end{cases} \tag{24}$$

Equations (22) and (23) were solved numerically. In order to carry out the calculations we have to specify the magnetic lattice pyramid and substrate as a simple cubic one. Results are presented graphically.

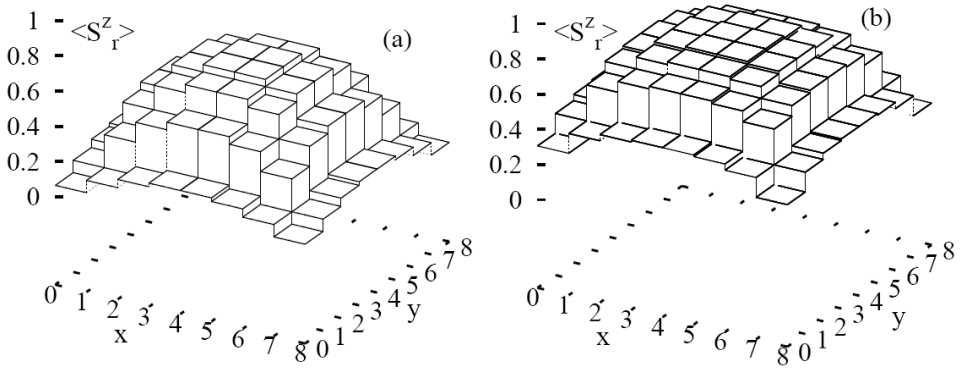

Fig. 2. Spatial distribution of magnetization in nanoscopic pyramid for $l = 4$, temperature $t = 4.2$, and $b = 2$, (a) without interaction with the substrate, $a = 0$, (b) for interaction parameter $a = 0.5$.

Figure 2 shows the spatial distribution of magnetization in the $l = 4$ layer of the nanoscopic pyramid for temperature $t = 4.2$ in relative units and $b = 2$: (a) without interaction with the ferromagnetic substrate $a = 0$, (b) for the interaction parameter of monoatomic layer $a = 0.5$. Figure 3 presents temperature dependence of the mean value of magnetization

$$X_l = \frac{\sum_{\boldsymbol{f}} X_{\boldsymbol{f}l}}{\sum_{\boldsymbol{f}}}, \tag{25}$$

with $X_{\boldsymbol{f}l}$ given by equation (22), for layers $l = 1, 2, 3, 4$ and parameters in (a) $a = 0$, $b = 1$ and in (b) $a = 0.5$, $b = 1$ (the pyramid not interacting with the substrate), where $\sum_{\boldsymbol{f}}$ denotes the number of spins in monoatomic layer l. The temperature dependence of the mean magnetization of the pyramid,

$$X = (4X_1 + 16X_2 + 36X_3 + 64X_4)/120, \tag{26}$$

is shown in Fig. 4.

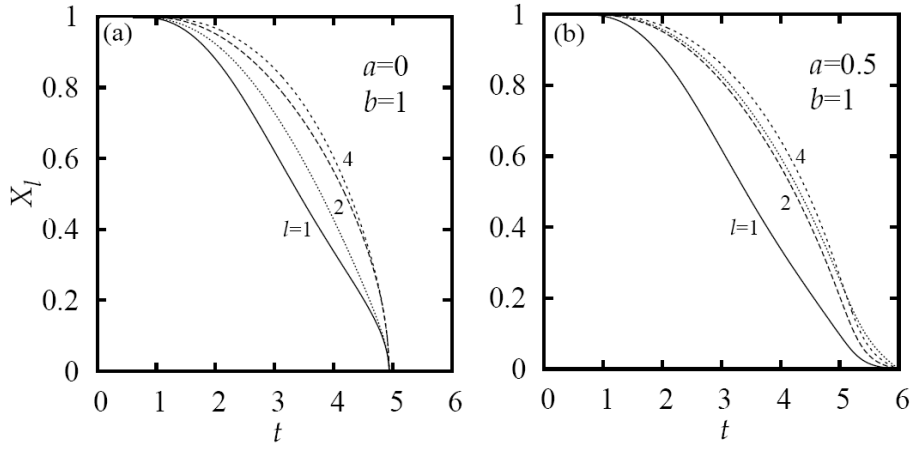

Fig. 3. Mean value of magnetization, $X_l = \sum_{\boldsymbol{f}l} X_{\boldsymbol{f}l} / \sum_{\boldsymbol{f}}$ in each monoatomic layer of pyramid, $l = 1, 2, 3, 4$, as a function of temperature t for $a = 0$, $b = 1$ (a), and $a = 0.5$, $b = 1.0$ (b).

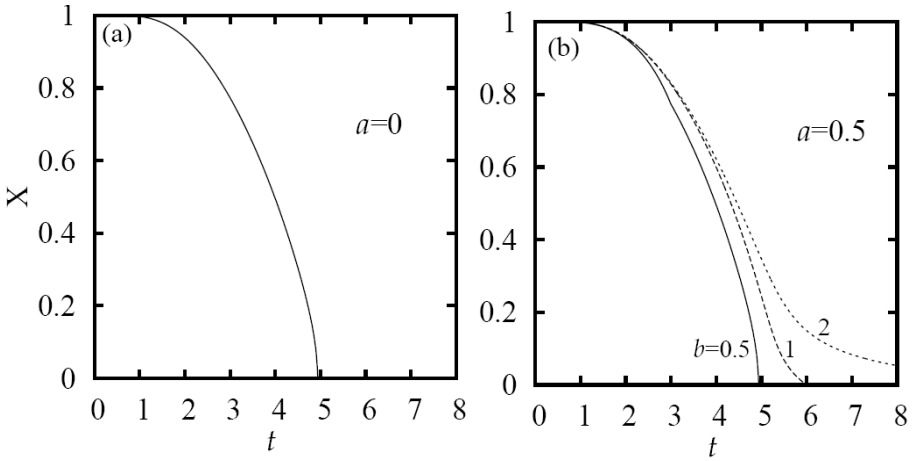

Fig. 4. Temperature dependence of the mean pyramid magnetization $X = (4X_1 + 16X_2 + 36X_3 + 64X_4)/120$ for $a = 0$ (a), and $a = 0.5$, $b = 0.5, 1, 2$ (b).

Finally, Fig. 5 presents magnetization y_r of monoatomic layers $r = 1, 2, 4, \infty$ of the ferromagnetic bulk substrate as a function of temperature t for $a = 0.1$ and $b = 0.5, 1, 2$. In Table the Curie temperature $t_{\rm c}$ of the ferromagnetic nanoscopic pyramid is given in relative units for different values of parameters a and b.

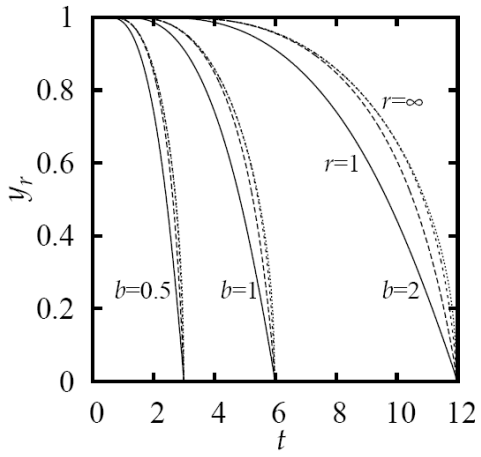

Fig. 5. Magnetization y_r of the monoatomic layer of the substrate versus temperature t, for $r = 1$ (continuous line), $r = 2, 4$ (dashed lines), and $r = \infty$ (dotted line).

TABLE

Curie temperature t_c (in relative units) for the nanoscopic pyramid.

a	b	t_c
0	arbitrary	4.93
0.1	0.5	4.93
0.1	1.0	5.99
0.1	2.0	11.95
0.5	1.0	5.99
0.5	2.0	11.95

4. Conclusions

The results we obtained lead us to the following conclusions:

- The interaction of a ferromagnetic nanoscopic pyramid with its bulk ferromagnetic substrate may have essential influence on the properties of the ferromagnetic pyramid;
- The Curie temperature t_c of the pyramid strongly depends on the Curie temperature of the bulk substrate;
- These results are illustrative in character and it would be difficult to verify them in an experiment;
- We believe that the reduced-state operator (4) may be successfully applied in studies of the influence of the bulk substrate on the thermodynamic properties of nonmagnetic systems and other more complex nanoscopic systems [5].

We expect that the development of the magnetic force microscope (MFM) method will enable at least some investigation of the spatial distribution of magnetization in nanoscopic pyramides. We intend to carry out calculations in a more realistic model of the substrate surface and the interface between the pyramid and the substrate. This can be done in the Gaussian fluctuation approximation (GFA)[6] or its modifications [7, 8].

Let us note that the reduced-state operator (4) couples the nanoscopic pyramid with the substrate. This means that the system does not have a finite number of spins. Therefore the use of e.g. Monte Carlo simulations would have little justification.

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