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Interface localization in thin ferromagnetic films

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Abstract. Interface localization in a thin ferromagnetic film with competing surface fields has been investigated by Monte Carlo simulation for an anisotropic Heisenberg model as a function of temperature and the anisotropy of the exchange interaction Λ. In the isotropic model limit, where $\Lambda \rightarrow 0$, no spontaneous magnetization of the film is observed and the magnetization profile across the film is antisymmetric, slowly varying from positive magnetization on one surface to negative on the other. However, in the limit $\Lambda \rightarrow 1$, when the model Hamiltonian is equivalent to that of the Ising model, a non-zero magnetization of the film is observed below a critical temperature T_c. This is associated with a localization of the interface between regions of positive and negative magnetization near the film surface and a degeneracy in the magnetization profiles exists between states of positive and negative total magnetization at low temperatures. The results of magnetic relaxation studies indicate that the magnetization decays exponentially with a relaxation time that increases with Λ and decreases with temperature.

1. Introduction

Interest in the area of thin magnetic films has been stimulated by progress in epitaxial growth techniques which allow ultrathin films of controllable thickness to be fabricated, and recent studies of thin magnetic films have revealed a number of novel phenomena that are not observed in the bulk materials. These result from the interplay of finite size effects arising from confinement and surface effects due to the competing surface fields. From the theoretical perspective the Ising model has been frequently and successfully adopted for the description of many characteristic features observed in thin magnetic films. However the Ising model of magnetism is founded on a very restricted representation of the magnetic spin orientation within the system and it is not *a priori* clear that this is appropriate for many magnetic materials, particularly in the restricted geometry of a thin film.

The classical Heisenberg model of magnetism represents one of the landmark physical descriptions of the magnetic properties of materials and its phase behaviour has attracted much investigation [1–4]. However, even when the associated model Hamiltonian is restricted to only isotropic exchange interactions between nearest neighbour spins, studies of the magnetic behaviour of the model are much more difficult than for the corresponding Ising model of magnetism, since, for the classical Heisenberg model, the ordering of the magnetic spins is very sensitive to the temperature and in the absence of an external field a spontaneous non-zero magnetization only occurs at zero temperature. The work of Taylor and Gyorffy [3] shows that in the absence of any anisotropy in the exchange interaction, there is no magnetic order at any finite non-zero temperature, the magnetic order being destroyed by long-wavelength spin waves [5, 6]. Unlike the magnetic spins in the Heisenberg model which can rotate through all possible orientations, in the Ising model the spins are

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restricted to orientations along a particular axis, conventionally denoted as the z-axis. For ferromagnetic exchange interactions in the Ising model, the spins order spontaneously below a critical temperature T_c even in the absence of an external field [7]. The order parameter for the ferromagnetic–paramagnetic phase transition in the Ising model is the spontaneous magnetization vector $\boldsymbol{M}$, which is zero for temperatures above T_c and non-zero below T_c [8].

The inclusion of an easy axis anisotropy in the Hamiltonian can significantly modify the properties of the Heisenberg spin system. Reproducing the phase behaviour of the Ising model for sufficiently strong anisotropies. Recent simulations [1–3] of ultra-thin films comprising a monolayer of Heisenberg spins with ferromagnetic exchange and magnetic dipole interactions show that with the inclusion of a single-site anisotropy the orientation of $\boldsymbol{M}$ is very sensitive to the anisotropy properties. The single-site anisotropy in these models constitutes a one-body, external field that prefers spin alignments perpendicular to the plane of the two-dimensional plane of the spins and minimizes the canting of the spins with increasing temperature. As shown by Taylor and Gyorffy [3], in the case of no single-site anisotropy ($\lambda = 0$) the model is equivalent to a classical Heisenberg spin system, while for large values of the single-site anisotropy ($\lambda \to +\infty$) the model reduces to an Ising model.

Binder *et al* [9–13] have made an extensive study of the thin ferromagnetic Ising film with competing surface forces which are external fields acting on the surfaces alone. Their work shows that the presence of competing surface forces can induce a phase transition in the bulk of the film. The competing surface fields favour a negative magnetization at one surface and a positive magnetization at the other surface. For sufficiently high temperatures the interface between the regions of negative and positive magnetization is centred on the middle of film, but it is not localized. The antisymmetric magnetization profile across the film results in a zero total magnetization of the film. However, for temperatures below a critical temperature $T_c(D)$ that depends on the film thickness, the interface becomes localized and is shifted from the centre toward the one of the surfaces. The particular surface depends on magnetization fluctuations in the bulk region and, most especially, the initial spin configuration. The low temperature magnetization profiles of the film $\boldsymbol{M}_n$ show a degeneracy between states of negative and positive total magnetization. In a recent paper [14], we presented a study of phase behaviour of the ferromagnetic Heisenberg spin system with single-site anisotropy in a thin film geometry under the action of competing surface fields. The interface localization transition seen in the thin ferromagnetic Ising film with competing surface fields can also be observed in the thin ferromagnetic Heisenberg film for sufficiently large values of the single-site anisotropy. However for small values of the single-site anisotropy the interface remained delocalized at all temperatures with zero total magnetization of the film. The critical temperature associated with the interface localization in the Heisenberg system is thus a function of both the film thickness and the single-site anisotropy λ, i.e. $T_c = T_c(\lambda, D)$. The interface localization transition observed in the Ising limit, $\lambda \to \infty$, disappears in the isotropic Heisenberg limit, $\lambda = 0$.

In two-dimensional Heisenberg spin systems, Binder and Landau [4] found that for ferromagnetic exchange interactions between pairs of nearest neighbour spins there was no spontaneous magnetization of the system at nonzero temperatures in the absence of any one-body external field, behaviour in marked contrast to the ferromagnetic–paramagnetic phase transition seen in the corresponding Ising spin systems with associated critical temperature T_c. However, if the Hamiltonian of the Heisenberg spin system was modified through the introduction of an anisotropy in the exchange interaction, Ising-like phase behaviour was observed for sufficiently large values of the exchange anisotropy. The anisotropic

exchange interaction of Binder and Landau leaves the spin–spin interaction between nearest neighbours unaltered in the z direction. But as the magnitude of the exchange anisotropy parameter is reduced from unity to zero, the contributions to the interaction energy from the components of the spin–spin interactions in the x and y directions reduce to zero. Thus the Hamiltonian for the anisotropic Heisenberg model smoothly interpolates between that of the isotropic Heisenberg model and the Ising model with the variation of the exchange anisotropy parameter Λ.

This paper investigates the phase behaviour and magnetization profiles of thin ferromagnetic films with competing surface fields in the anisotropic Heisenberg model as a function of the anisotropy of the exchange interaction and temperature. In the following section a full description of the model is given and the details of the Monte Carlo simulation method are presented. The equilibrium phase behaviour of the model system as a function of the exchange anisotropy and the temperature are discussed in sections 3 to 5. The temperature dependence of the magnetic relaxation is investigated in section 6 and the paper concludes with a summary of the key findings.

2. The model

The system under consideration is a three-dimensional ferromagnetic thin film of finite thickness D that is described by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}[(1-\Lambda)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] - \sum_{i\in\text{surface }1} \boldsymbol{H}_1\cdot\boldsymbol{S}_i - \sum_{i\in\text{surface }D} \boldsymbol{H}_D\cdot\boldsymbol{S}_i \qquad (1)$$

where $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ is a classical Heisenberg spin (three-dimensional unit vector) at lattice site i. The notation $\langle i, j\rangle$ denotes that the summation is restricted to nearest-neighbour pairs of Heisenberg spins, each pair being counted only once. J is a coupling constant characterizing the magnitude of the exchange interaction and for ferromagnets $J > 0$. Following Binder and Landau [4], Λ determines the strength of the exchange anisotropy and is only applied to components of the exchange interaction in the x and y directions. For $\Lambda = 0$, we return the isotropic limit when the model Hamiltonian is identical to that for a classical Heisenberg spin system, while for $\Lambda = 1$, the Hamiltonian reduces to that of the Ising model. $\boldsymbol{H}_1$ and $\boldsymbol{H}_D$ are the applied surface fields.

We consider a simple cubic lattice of size $L\times L\times D$, in units of the lattice spacing, and apply periodic boundary condition in the x and y directions. Free boundary conditions are applied in the z direction which is of finite thickness D. The system is subject to competing surface fields applied to layers $n = 1$ and $n = D$ of the film with

$$\boldsymbol{H}_1 = h\hat{\boldsymbol{z}}\delta_{i1} \qquad (2)$$

$$\boldsymbol{H}_D = -h\hat{\boldsymbol{z}}\delta_{iD} \qquad (3)$$

giving a Hamiltonian

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}[(1-\Lambda)(S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z] - h\left(\sum_{i\in\text{surface }1} S_i^z - \sum_{i\in\text{surface }D} S_i^z\right). \qquad (4)$$

A film thickness $D = 12$ and surface field strength $h = -0.55$ were used throughout and the simulations performed for lattices of size $L = 32$. The Metropolis algorithm [15] was used in the Monte Carlo simulations with trial configurations generated from Barker–Watts [16] spin rotations. The magnitude of the maximum spin rotation was adjusted to ensure

approximately 50% of trial configurations were rejected in the bulk equilibrium state. The z component of the magnetization for the film

$$M_z = \frac{1}{D}\sum_{n=1}^{D} M_n^z \tag{5}$$

and the z component of the magnetization for the nth layer of the film

$$M_n^z = \frac{1}{L^2}\sum S_i^z \tag{6}$$

were determined for different values of the exchange anisotropy Λ and temperature T. The fluctuations in the magnetization were used to calculate the layer susceptibility χ_n which is given by

$$\chi_n = L^2\left(\langle M_n^{z2}\rangle - \langle M_n^z\rangle^2\right)/k_BT \tag{7}$$

where k_B is Boltzmann's constant. Simulations were performed for up to 10^6 Monte Carlo steps per spin (MCS/spin) to ensure equilibration of systems in the Heisenberg limit ($\Lambda = 0$) [4]. Equilibrium averages were typically taken over 2×10^5 MCS/spin with initial transients ignored. For systems in the Ising limit ($\Lambda = 1$), much shorter runs could be performed.

3. Exchange anisotropy and interface localization

The approach to equilibrium of the z component mean magnetization per spin, $\langle M_z\rangle$, for different values of Λ from $\Lambda = 0$ to $\Lambda = 1$ obtained from the simulations at a reduced temperature of $T^* = k_BT/J = 1.0$ are shown in figure 1. In each case the initial spin configuration corresponded to an ordered state with initially spin $S_i^z = +1$ for all i and MCS/spin is used as a unit of time. For the film in the Ising limit $\Lambda = 1$, the system quickly approaches an equilibrium state of non-zero magnetization. However, for an isotropic spin–spin interaction $\Lambda = 0$, the Heisenberg spins continuously rotate to reach equilibrium at zero magnetization of the film. No spontaneous magnetization is observed even though $T < T_c(D)$ for the Ising system $T^* = 4.0$ [12]. The model is a classical Heisenberg spin system and the ordered spin states are quickly destroyed at finite temperature. However small increases in the size of the exchange anisotropy show a dramatic change in the magnetization of the film. For $\Lambda = 0.110$, the temporal evolution of the magnetization per spin closely resembles that of the Ising-like spin system with $\Lambda = 1$. But for $\Lambda = 0.090$, the temporal evolution of the spin system is significantly altered and closely resembles the isotropic Heisenberg spin system with $\Lambda = 0$. When a spontaneous magnetization of the film persists, the magnitude of the equilibrium magnetization of the film decreases with Λ. Another notable feature of the time evolution of the magnetization is large fluctuations in $\langle M_z\rangle$ for $\Lambda = 0.090$. These arise in Heisenberg spin systems since the probability of spin flips becomes very small and metastable states occur due to strong magnetization in the x and y directions which averages to zero much more quickly than for $\langle M_z\rangle$ [4].

The magnetization profiles across the film, M_n^z, for different Λ at a temperature $T^* = 1.0$ are shown in figure 2(a). The figure shows results from simulations of an initial spin state of $S_i^z = +1$ for all i. A qualitative difference between the results for the $\Lambda = 0$ and $\Lambda = 1$ spin systems is immediately apparent. For the isotropic system with $\Lambda = 0$, the interface between regions of negative and positive magnetization is not localized and the point of zero magnetization is located at the centre of the film. However for the Ising Hamiltonian with $\Lambda = 1$, the interface disappears into the film surface. Since $M_n^z > 0$ for all n, a large

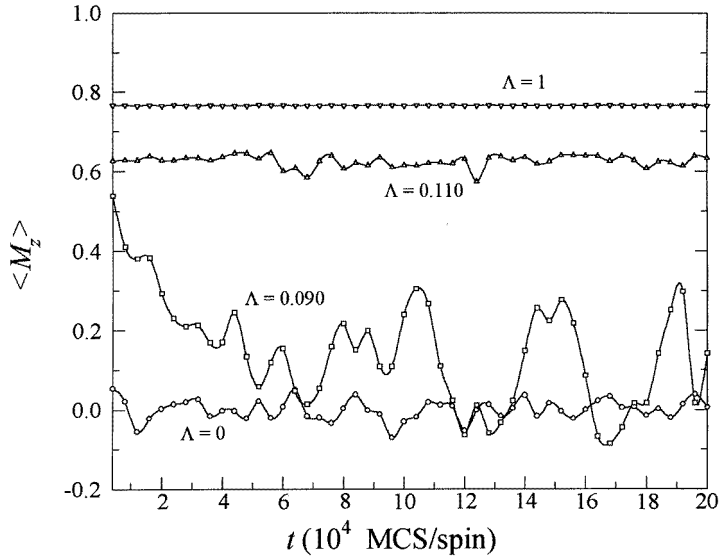
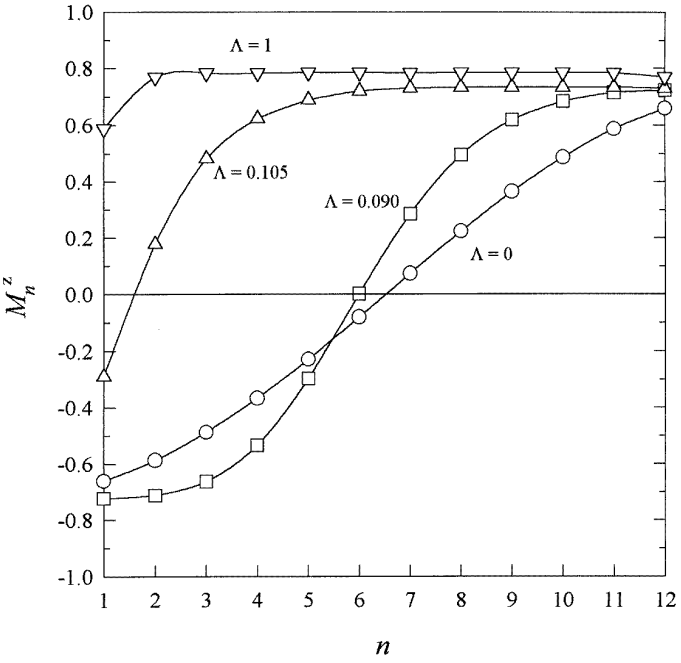


Figure 1. Mean magnetization per spin, $\langle M_z \rangle$, against time, in units of Monte Carlo steps per spin, for thin ferromagnetic Heisenberg films of size $32 \times 32 \times 12$ with different values of the exchange anisotropy in the range $0 \leqslant \Lambda \leqslant 1$. All results were obtained from an initial spin state of $S_i^z = +1$ for all i at a temperature $T^* = 1.0$. The curves through the points are only guides to the eye.

value of the film magnetization results. For $0 < \Lambda < 1$, the interface is seen to move from the centre toward the surface with increasing Λ, but not gradually. For $\Lambda = 0.090$, the profile of M_n^z across the film is similar to that of the isotropic Heisenberg spin system with $\Lambda = 0$. However, following a small increase of Λ to $\Lambda = 0.105$, the layer magnetization profile is seen to resemble that of the Ising-like spin system with $\Lambda = 1$. To investigate the spin behaviour in more detail in the transition region, plots of M_n^z for a temperature $T^* = 1.0$ are presented in figure 2(b) for $0.095 < \Lambda < 0.100$. For the sake of clarity the figure shows results from $\Lambda = 0.096$, 0.100 with an initial state of $S_i^z = +1$ for all i and with an initial state of $S_i^z = -1$ for $\Lambda = 0.095$, 0.099, 0.103. The figure shows the surface fields locally constrain the spins to align in the negative direction near one surface and in the positive direction near the other surface. In the bulk, the mean spin orientation of the layers varies smoothly from one surface to the other. For $\Lambda = 0.095$, the point of zero magnetization in the profile is located in the middle of the film. But as Λ increases the magnetization profile becomes asymmetric with the point of zero magnetization shifted toward the surface of the film. This produces a non-zero value of the film magnetization. The direction of the interface displacement depends on the initial spin configuration and a degeneracy exists between states of positive and negative total magnetization.

Figure 3 shows the film profiles of susceptibility χ_n across the film at a temperature $T^* = 1.0$ over the transition region with $\Lambda = 0.096$, 0.099, 0.101 from an initial configuration of $S_i^z = -1$ for all i. The figure shows peaks in the susceptibility across the film and the peaks in χ_n for each Λ are located in the same layer as the point of zero magnetization in the profiles of M_n^z, indicating larger fluctuations of spins in the interface between regions of positive and negative magnetization.



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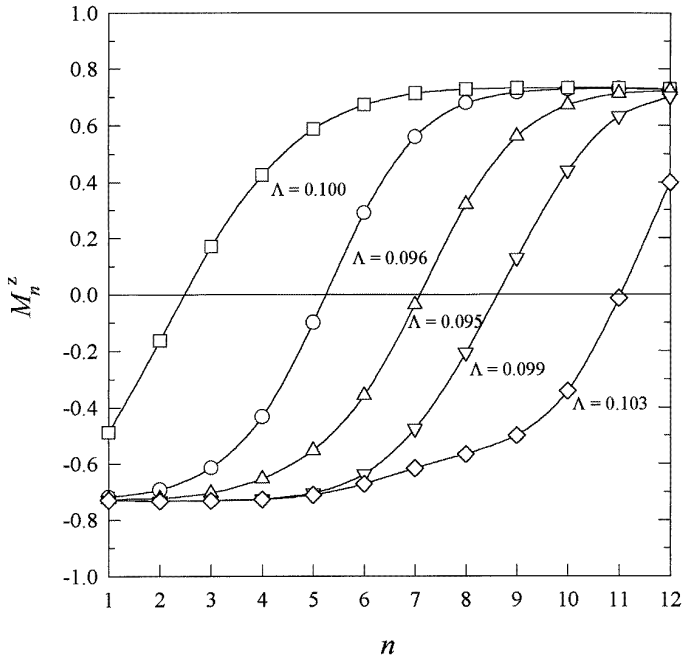


(b)

Figure 2. Magnetization profiles across the film, M_n^z, against layer number n for $D = 12$ with surface fields $H_1/J = -H_D/J = -0.55$ at a temperature $T^* = 1.0$: (a) from an initial spin state of $S_i^z = +1$ for all i and (b) $S_i^z = +1$ for $\Lambda = 0.096$, 0.100 and $S_i^z = -1$ for $\Lambda = 0.095$, 0.099, 0.103.

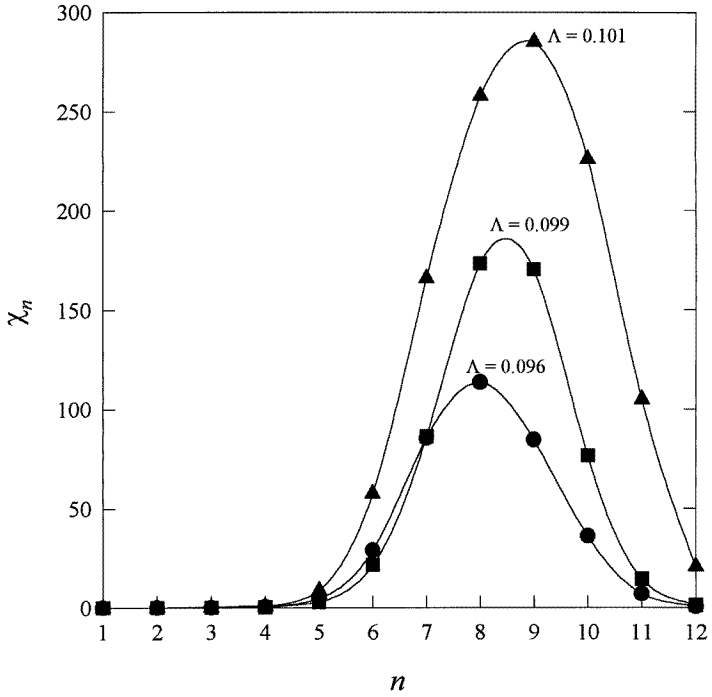


Figure 3. Layer susceptibility χ_n against layer number n for $D = 12$ at a temperature $T^* = 1.0$ from an initial spin state of $S_i^z = -1$ for all i. The curves drawn are only guides to the eye.

4. Temperature dependence of the phase behaviour

The temperature dependence of the magnetization profiles across the film is shown in figure 4 for an exchange anisotropy of $\Lambda = 0.1$. Once more for clarity an initial state of $S_i^z = +1$ for all i is used at temperatures $T^* = 0.9$, 1.0, 1.1, while an initial state of $S_i^z = -1$ for all i is used at temperatures $T^* = 0.7$, 1.4. At the highest temperature $T^* = 1.4$, we find that the interface is not localized and the point of zero magnetization is located in the centre of the film, between layers $n = 6$ and $n = 7$. The mean film magnetization $\langle M_z \rangle$ is zero due to the symmetry of M_n^z about the middle of the film. However, as the temperature is reduced from $T^* = 1.1$ to 0.7, the interface becomes increasingly more localized and is shifted toward the surface with again a degeneracy between two states of the film magnetization. The selected state once more depends on the initial spin configuration. The film has a non-zero value of $\langle M_z \rangle$ at these temperatures which increases with decreasing T^*. This behaviour can be regarded as a remnant of the Ising model behaviour seen by Binder *et al* [11–13]. When $\Lambda = 0$, the model becomes a classical Heisenberg spin system which has no spontaneous magnetization at a non-zero temperature and the interface between negative and positive magnetization is always located in the centre of the film.

In order to study the dependence on Λ of the critical temperature $T_c(\Lambda, D)$, simulations have been performed to determine $\langle M_z \rangle$ as a function of temperature for different values of the exchange anisotropy, in this case $\Lambda = 0.1$, 0.2, 0.5 and 1. For $\Lambda = 0$, although not shown in figure 5, we have $T_c^*(0, D) = 0$. The film shows no spontaneous magnetization with $\langle M_z \rangle = 0$ for all T^*. As expected, the critical temperature $T_c(\Lambda, D)$ increases as Λ

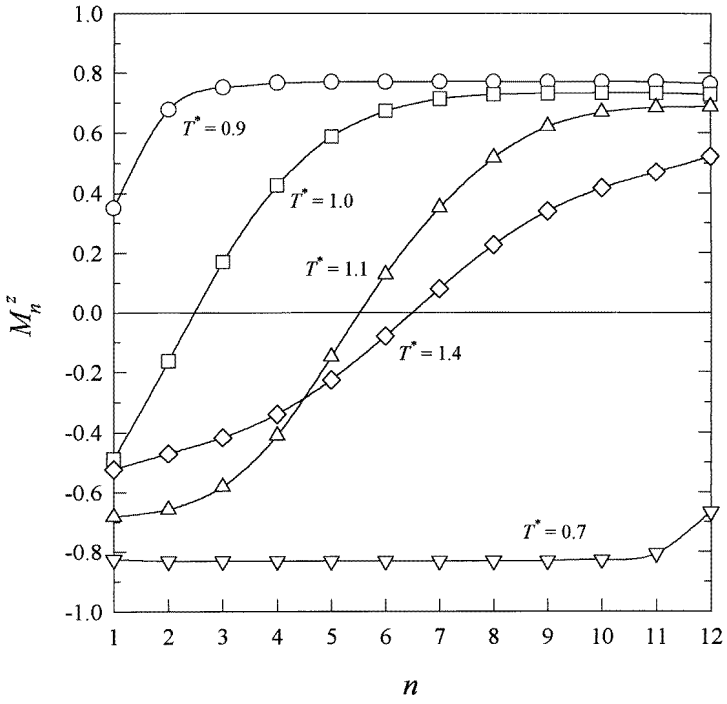


Figure 4. Magnetization profiles across the film, M_n^z, against layer number n, for $D = 12$ with $\Lambda = 0.1$ at different temperatures with surface fields $H_1/J = -H_D/J = -0.55$. An initial spin state of $S_i^z = +1$ for all i was used for $T^* = 0.9$, 1.0, 1.1, while an initial spin state of $S_i^z = -1$ for all i was used for $T^* = 0.7$, 1.4.

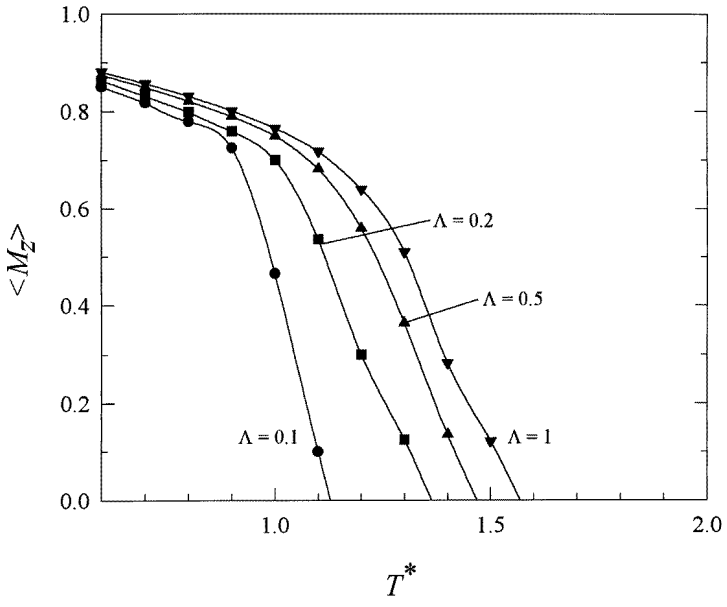


Figure 5. Temperature dependence of mean magnetization per spin, $\langle M_z \rangle$, for different values of the exchange anisotropy Λ from an initial spin state of $S_i^z = +1$ for all i.

increases from 0.1 to 1. For $T > T_c$ the film shows no spontaneous magnetization with $\langle M_z \rangle = 0$, while for $T < T_c$ spontaneous magnetization with $\langle |M_z| \rangle > 0$ is observed. However, for the system with the Ising Hamiltonian, $\Lambda = 1$, we find that $T_c^*(\Lambda = 1, D = 12) \cong 1.5$ is not equivalent to that of the Ising spin system $T_c^*(D = 12) = 4.0$ [12]. This discrepancy in T_c arises from the magnitude of the z component of spin in the simulation. The model definition of the Ising spin system requires $|S_z| = 1$, while in the Heisenberg spin system used here $0 \leqslant |S_z| \leqslant 1$ even in the Ising limit of the Hamiltonian $\Lambda = 1$. This gives a lower value of T_c than that obtained by Binder *et al* for Ising spins.

A value for T_c closer to the value of $T_c^*(D = 12) = 4.0$ found for the Ising spin system can be obtained by the addition of a single-site anisotropy term, $-\lambda \sum_i (S_i^z)^2$, to the Hamiltonian of equation (4). In the limit of $\lambda \to \infty$, the model reduces to an Ising spin system, since the additional quadratic term in the Hamiltonian forces the spins to align along the z-axis. Figure 6 shows the results of $\langle M_z \rangle$ in the Heisenberg spin system with $\Lambda = 1$ as a function of the single-site anisotropy λ at $T^* = 2.0$ and $T^* = 3.0$. In the figure, the dotted horizontal line indicates the value of $\langle M_z \rangle$ for an Ising spin system at $T^* = 2.0$. The figure shows that for $T^* = 2.0$, we have $\langle M_z \rangle = 0.76$ with $\lambda = 6$. Results for $T^* = 3.0$ show that, for higher temperatures, much larger values of λ are needed to generate high values of $\langle M_z \rangle$. Although not shown in the figure, for $T^* = 3.5$ we have $\langle M_z \rangle = 0.55$ with $\lambda = 100$. In all cases, for $\lambda \to \infty$ the results of the Heisenberg spin system reduce to those of the Ising spin system as required.

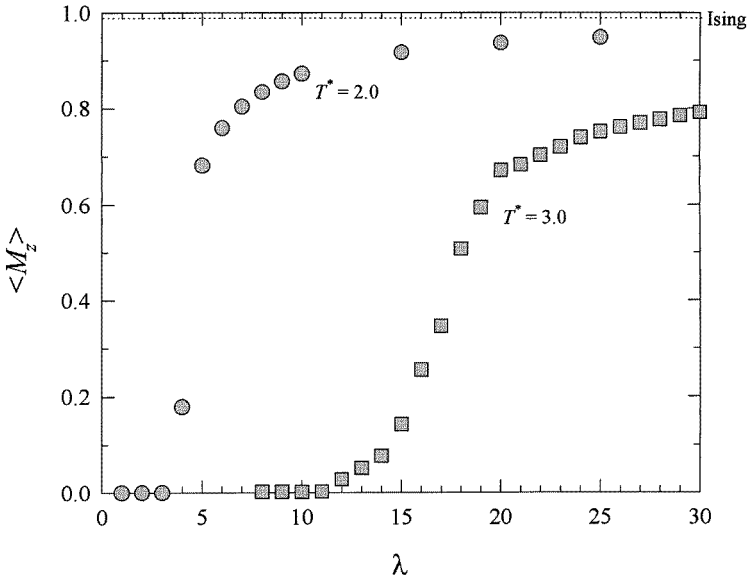


Figure 6. Variation of mean magnetization per spin, $\langle M_z \rangle$, for different values of the single-site anisotropy λ at temperatures of $T^* = 2.0$ and 3.0. The dotted line indicates the result for an Ising spin system at $T^* = 2.0$.

5. Spin orientation

The work of the previous section showed that the critical temperature $T_c(\Lambda, D)$ of the anisotropic Heisenberg film increases with Λ. However, in the Ising limit of the

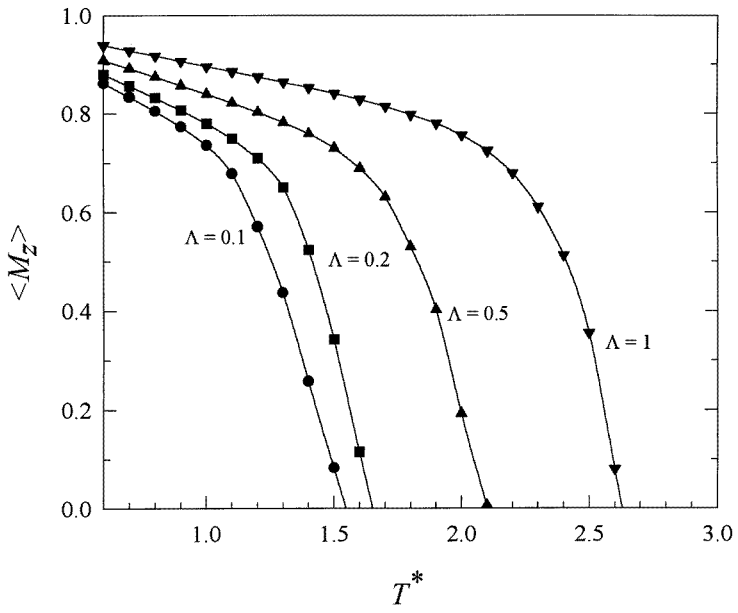
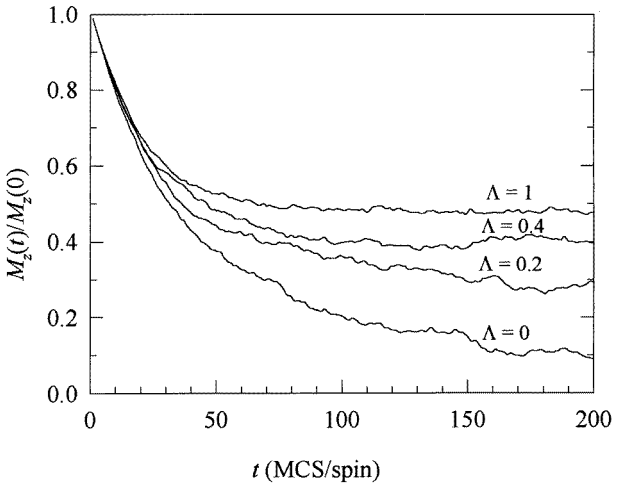


Figure 7. Temperature dependence of mean magnetization per spin, $\langle M_z \rangle$, for different values of the exchange anisotropy Λ from an initial spin state of $S_i^z = +1$ for all i obtained when an orientational spin flip is included in the generation of the trial configuration.

Hamiltonian, we find that $T_c^*(\Lambda = 1, D = 12)$ is not equivalent to that of the Ising spin system. To recover Ising behaviour a sufficiently strong single-site anisotropy term must be included in the Hamiltonian that forces the spins to align along the z-axis. However the $M_z(\lambda)$ curve shown in figure 6 has an interesting characteristic shape for all T^*. At small λ the addition of the uniaxial external field has little effect. But for a sufficiently large value of λ, M_z rises sharply with increasing λ. This threshold value for λ is temperature dependent. It is further interesting to note a distinct change in gradient of the $M_z(\lambda)$ curve that occurs for values of λ above the threshold value at $\lambda \approx 6$ for $T^* = 2.0$ and $\lambda \approx 20$ for $T^* = 3.0$.

To investigate this aspect of the system behaviour in more detail the simulation algorithm was modified to incorporate a trial spin rotation called the orientational spin flip. In the modified algorithm the trial spin orientation is generated by the usual Barker–Watts [16] spin rotation followed by an orientational spin flip in which the direction of the spin is first reversed and then reoriented along the z-axis. The orientational spin flip is accepted if a random number R uniformly generated on the interval $[0, 1]$ satisfies $R < \Lambda/2$. Thus the likelihood of an orientational spin flip contributing to generation of the trial spin configuration is proportional to the magnitude of the anisotropy Λ. The trial configuration is accepted or rejected on the basis of the standard Metropolis criterion. The orientational spin flip encourages spin alignment along the z-axis and gives a higher value of $|S_z|$ at any given temperature. The results from a set of simulations with the orientational spin flip for the same set of system parameters as used in figure 5 are shown in figure 7. Comparison of the results of figures 5 and 7 show that as might be expected the critical temperatures $T_c(\Lambda, D)$ obtained with the orientational spin flip are closer to the Ising values for any given Λ. In particular we find that $T_c^*(\Lambda = 1, D = 12) \cong 2.6$ for simulations with the orientational spin flip, as compared to $T_c^*(\Lambda = 1, D = 12) \cong 1.6$ for the standard Heisenberg model simulations.



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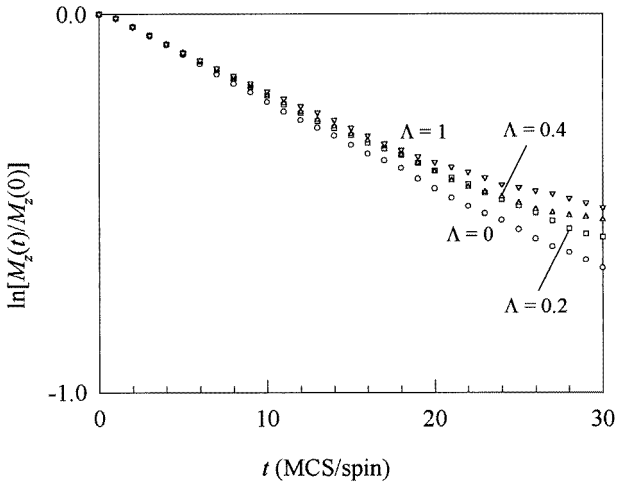
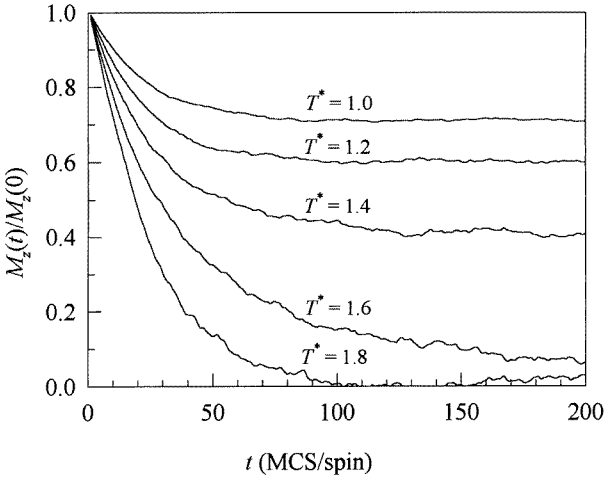


(b)

Figure 8. Relaxation of the film magnetization with time for different values of Λ with zero surface field at a temperature $T^* = 1.5$: (a) reduced magnetization $M_z(t)/M_z(0)$ against time and (b) $\ln[M_z(t)/M_z(0)]$ against time.

This is closer to the value of $T_c^*(D = 12) = 4.0$ obtained for the Ising spin system.

Further simulations with the orientational spin flip show that for $\Lambda = 1$ and $T^* = 2.0$ a value of $\langle M_z \rangle = 0.76$ is obtained. This is the same as that found in the conventional simulations on the anisotropic Heisenberg spin system with $\Lambda = 1$ and a single-site anisotropy $\lambda = 6$. Indicating that for $T^* = 2.0$ an external field strength of $\lambda = 6$ is required to essentially orient the Heisenberg spins along the z-axis. Additional increases in λ only serve to dampen out the small fluctuations in the spin orientation from the z-axis. Similar behaviour is also observed for $T^* = 3.0$. Thus the change in gradient of $M_z(\lambda)$ that occurs for a value of λ above the threshold value can be associated with the ordering of the Heisenberg spins along the z-axis. Ising behaviour is fully recovered when all fluctuations in spin orientation from the z-axis are eliminated in the limit of $\lambda \to \infty$.



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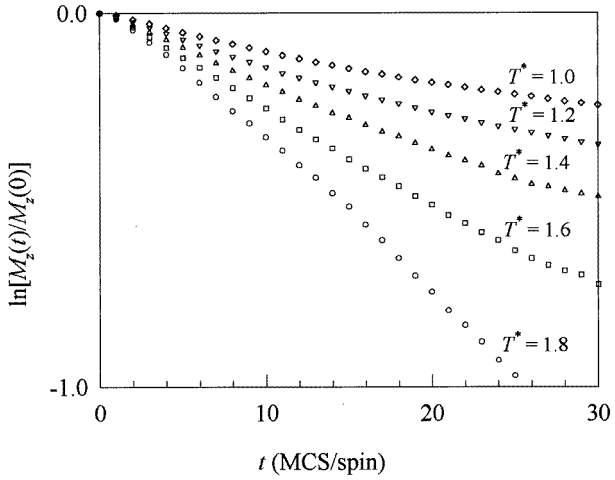

(b)

Figure 9. Relaxation of the film magnetization with time for $\Lambda = 0.1$ with different temperatures and zero surface field: (a) reduced magnetization $M_z(t)/M_z(0)$ against time and (b) $\ln[M_z(t)/M_z(0)]$ against time.

6. Magnetic relaxation

The time dependence of the magnetic relaxation is investigated here for different values of Λ and temperature. In these studies, the trial configurations were generated by the Barker–Watts spin rotation of randomly selected spins with a magnitude of the maximum spin rotation adjusted to ensure half of the trial configurations were rejected in the equilibrium state. No orientational spin flip was used. As elsewhere [17], we focus on the role of Λ and temperature in determining the relative magnetic relaxation behaviour of the Heisenberg spin systems and do not attempt to obtain absolute relaxation times. In figure 8(a), for different Λ from $\Lambda = 0$ to $\Lambda = 1$, the ratio of time dependent magnetization to the initial magnetization,

$M_z(t)/M_z(0)$, is shown as a function of time at temperature $T^* = 1.5$ for $h = 0$ from an initially ordered state with $S_i^z = +1$ for all i. Comparison with the results in figure 1 for a similar system with $h = -0.55$ shows that equilibrium was obtained in a shorter time for $h = 0$. In general the relaxation time increases with the surface field. The results of figure 8(a) also show a faster decay of the initial state is observed for smaller Λ but that the time required to achieve the equilibrium is increased. For $\Lambda = 1$, in the Ising limit, a much shorter time is required to reach an equilibrium and produce a finite value of magnetization. Figure 8(b) shows the magnetic relaxation on a natural logarithm scale, $\ln[M_z(t)/M_z(0)]$, as a function of time for different Λ. The linear character of the curves for short times indicates that the initial magnetic relaxation can be characterized by an exponential decay and the magnetic relaxation can be written as

$$\frac{M_z(t)}{M_z(0)} = \exp\left(\frac{-t}{\tau(\lambda, T)}\right) \tag{8}$$

where τ is a relaxation time. Table 1 gives the relaxation times for different values of Λ at $T^* = 1.5$ corresponding to the systems in figure 8 with error estimates obtained from ten repetitions with different random number sequences. It is interesting to note that the dramatic change in the equilibrium magnetization profile of the film observed for $\Lambda \sim 0.1$ is not mirrored in the relaxation behaviour that shows a continuous gradual change of τ with Λ.

Table 1. Relaxation time τ for the thin Heisenberg film with $D = 12$, temperature $T^* = 1.5$ and zero surface field $h = 0$ for exchange anisotropy Λ.

Λ	τ (MCS/spin)
0	45.8 ± 0.2
0.2	52.4 ± 0.5
0.4	57.3 ± 0.3
1	64.1 ± 0.6

The temperature dependence of the magnetic relaxation is shown in figure 9(a) for $\Lambda = 0.1$. Again the decay of the magnetization is monitored for $h = 0$ with an initial state of $S_i^z = +1$ for all i. The rate of decay of the initial state is greater for higher temperatures, but the time to achieve equilibrium also increases with temperature. Once more the initial magnetic relaxation is governed by an exponential decay as shown in figure 9(b). Table 2 gives the relaxation times for $1.0 \leqslant T^* \leqslant 1.8$ at $\Lambda = 0.1$ corresponding to the systems in figure 9 with error estimates obtained from ten repetitions with different random number sequences. Once more the relaxation time varies smoothly through the interface delocalization transition which occurs in this system for $T^* \sim 1.5$.

Table 2. Relaxation time τ for the thin Heisenberg film with $D = 12$, exchange anisotropy $\Lambda = 0.1$ and zero surface field $h = 0$ at temperature T^*.

T^*	τ (MCS/spin)
1.0	131.8 ± 0.7
1.2	91.2 ± 0.4
1.4	61.4 ± 0.4
1.6	39.3 ± 0.2
1.8	24.9 ± 0.2

7. Conclusions

We have studied the phase behaviour of thin ferromagnetic films with competing surface fields within an anisotropic Heisenberg model. The exchange anisotropy Λ in the Hamiltonian is clearly seen to be an important factor in controlling the phase behaviour of the film. For $\Lambda = 0$, the isotropic model is equivalent to a classical Heisenberg spin system which shows no spontaneous magnetization for $T > 0$. However for small increases in Λ, the model yields qualitative behaviour previously observed within the corresponding Ising model by Binder *et al* with a spontaneous magnetization of the film at low temperatures. However, the Ising limit $\Lambda = 1$ of this model does not quantitatively agree with other studies on the thin Ising film. For although the model Hamiltonians used were identical, in the present model the spins were still free to rotate through all orientations, whereas in the Ising simulations the spins are restricted to orientations in the z direction alone. Full correspondence with the Ising system could be obtained through the introduction of an additional external field, the single-site anisotropy λ, into the Hamiltonian. The critical temperature T_c characterizing the phase behaviour of the magnetization of the film strongly depends on the magnitude of Λ as does the magnetic relaxation time τ.

These observations can be expected to be of relevance in studies of the phase behaviour and dynamics of thin films of more complex materials such as ferronematic liquid crystals. These systems can also be represented by a continuous spin model and show spontaneous ordering at low temperatures, but have more complicated Hamiltonians.

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