Phase behaviour of the antiferromagnetic plane rotator model

2002 J. Phys.: Condens. Matter 14 7155

(http://iopscience.iop.org/0953-8984/14/30/306)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 7155–7163 PII: S0953-8984(02)35614-5

Phase behaviour of the antiferromagnetic plane rotator model

A M Abu-Labdeh[1], N P Chafe[1], J P Whitehead[1,4], K De'Bell[2] and A B MacIsaac[3]

[1] Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St John's, Newfoundland, Canada A1B 3X7
[2] Department of Mathematical Sciences, University of New Brunswick at Saint John, Saint John, New Brunswick, Canada E2L 4L5
[3] Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada N6A 5B9

Received 8 April 2002
Published 17 July 2002
Online at stacks.iop.org/JPhysCM/14/7155

Abstract

The phase diagram of an ultrathin film of magnetic rotors confined to the plane of the film has been determined from Monte Carlo simulations. In this square lattice system, the classical spins interact through a nearest neighbour antiferromagnetic exchange and the dipolar interactions. The phase diagram shows a dipolar antiferromagnetic phase for low values of $|J|/g$, and a simple antiferromagnetic phase for large values of $|J|/g$. The Monte Carlo data also indicate that the dipolar phase separates into two distinct phases for different values of $|J|/g$. In the first phase the spins are aligned along the x- or y-axis, while in the second phase the sublattice magnetization is oriented at $\pi/4$ to the x- and y-axis. The results for the plane rotator model are compared with previous results obtained for the Heisenberg model, which showed an analogous phase behaviour. This comparison clarifies the role played by out-of-plane degree of freedom and provides some further insight into this intriguing transition.

1. Introduction

The properties of ultrathin magnetic films and other quasi-two-dimensional systems remain of considerable interest. This interest arises in part from the insight they provide into the effects that can arise as a consequence of the subtle interplay between the long ranged anisotropic dipolar interactions, the short ranged exchange interactions and the on-site surface anisotropy [1]. Additional interest arises from the technological applications of such systems such as data storage [2–4] where, for example, antiferromagnetic layers are used to pin ferromagnetic layers in certain magnetic multilayered structures. Fundamental studies of

[4] Author to whom any correspondence should be addressed.

these properties are helpful in determining whether the magnetic structures and their associated equilibrium properties are suitable for such applications.

In a previous paper [5] (hereafter referred to as I), results from a series of Monte Carlo simulations were presented for the case of a two-dimensional film of magnetic moments arranged on a square lattice interacting through both an antiferromagnetic exchange interaction and a dipolar interaction. In this model the magnetic moments were represented by three-dimensional vectors of fixed magnitude. This model represents an important limiting case of a more general model which includes the on-site surface anisotropy. In I, it was found that the system exhibits a reorientation transition from an in-plane antiferromagnetic phase to an out-of-plane antiferromagnetic phase as the magnitude of the exchange coupling is increased. In addition the in-plane antiferromagnetic ordering exhibits two phases; in one the moments are aligned parallel to the square lattice axes, in the other the staggered magnetization is rotated by $\pi/4$ relative to the square lattice axes.

The appearance of the in-plane magnetic order in these systems is a subtle effect since the planar ground state is continuously degenerate despite the anisotropic nature of the dipolar interaction [6]. The magnetic order arises as a consequence of the disorder created by the thermal fluctuations [5, 6], and provides an explicit example of the 'order from disorder' [7, 8] phenomenon which is known to give rise to magnetic ordering in a number of frustrated magnetic systems [9, 10]. Earlier theoretical studies on a truncated dipole-like interaction have shown that both thermal fluctuations and dilution can stabilize the antiferromagnetic state, with thermal fluctuations favouring ordering along the lattice axis and dilution favouring ordering aligned at $\pi/4$ to the lattice axis [8, 11]. In I it was argued that thermally activated isolated out-of-plane spin flips would create a disorder similar to the effects of dilution, with a density controlled by the strength of the exchange interaction J and the temperature T. It was therefore conjectured that these spin flips were the cause of the in-plane reorientation. The present work was initiated to examine this conjecture since the out-of-plane spin flips are absent in the plane rotator model. The current study is also of interest as it may be considered to be another limiting case of the more general model that includes the on-site surface anisotropy. In this limit the magnitude of the on-site anisotropy is effectively infinite and restricts the moments to be in plane so that they may be treated as strictly planar rotors.

In this paper we shall concentrate on differences and similarities between the results for this plane rotator model and the model studied in I, and address the question posed above. The results reported here are primarily based on Monte Carlo simulations of the square lattice model with Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j + g \sum_{i \neq j} \left(\frac{\vec{\sigma}_i \cdot \vec{\sigma}_j}{r_{ij}^3} - 3 \frac{(\vec{\sigma}_i \cdot \vec{r}_{ij})(\vec{\sigma}_j \cdot \vec{r}_{ij})}{r_{ij}^5} \right) \tag{1}$$

where $\{\vec{\sigma}_i\}$ denote the set of two-dimensional unit vectors that describe the orientation of the magnetic moments at the lattice sites $\{\vec{r}_i\}$ and lie in the plane of the lattice. Results are reported for several lattice sizes in the range $N = 32 \times 32$ to 104×104. Periodic boundary conditions are imposed on the spin configurations and the dipolar interactions are evaluated using the Ewald summation technique. The simulations are done using the standard Metropolis algorithm. Throughout the exchange interaction is assumed to be antiferromagnetic (i.e. $J < 0$). For the results reported in the current work an equilibration time of 10×10^3 Monte Carlo steps (MCSs) was used for each simulation, while the averaging was performed using samples taken every ten MCSs. The number of samples used to calculate the averages, however, depended on both the size of the system and the temperature, and ranged from from 10×10^3 samples at high temperature for the 104×104 system to 29×10^3 samples at low temperature for the 32×32 system.

As in I, we decompose the square lattice into four sublattices, each labelled by an index $\alpha = 1, 2, 3, 4$, and define for each sublattice a corresponding sublattice magnetization

$$\vec{M}^{\alpha} = \frac{4}{N}\left(\sum_{\vec{r}_\alpha} \sigma^x(\vec{r_\alpha})\right)\hat{x} + \frac{4}{N}\left(\sum_{\vec{r}_\alpha} \sigma^y(\vec{r_\alpha})\right)\hat{y}. \tag{2}$$

From these sublattice magnetizations we construct two order parameters:

$$\vec{M}_{AF} = \tfrac{1}{4}[(M_x^1 + M_x^2 - M_x^3 - M_x^4)\hat{x} + (M_y^1 + M_y^3 - M_y^2 - M_y^4)\hat{y}] \tag{3}$$

and

$$\vec{M}_{AA} = \tfrac{1}{4}[(M_x^1 + M_x^4 - M_x^3 - M_x^2)\hat{x} + (M_y^1 + M_y^4 - M_y^3 - M_y^2)\hat{y}]. \tag{4}$$

The first of these order parameters, $\vec{M}_{AF}$, characterizes ordering in the manifold of ground states of the pure dipolar system ($J = 0$) [6]. We denote these states as AF states. It can be shown that the second order parameter, $\vec{M}_{AA}$, is zero in these states. The second order parameter, $\vec{M}_{AA}$, characterizes ordering in the ground states corresponding to the antiferromagnetic states in which each nearest neighbour pair is aligned antiparallel. We denote these states as AA states. It can be shown that the first order parameter, $\vec{M}_{AF}$, is zero in these states.

2. The phase diagram

At zero temperature, for $|J| < J_0$ ($J_0/g = 3.2109$) the AF phase is energetically favoured, while for $|J| > J_0$ the AA phase is energetically favoured. This may be compared with the value of the exchange constant $|J|/g = 1.2265$ at which the moments switch from in-plane AF ordering to out-of-plane AA ordering in the case of the Heisenberg model studied in I.

At finite temperature the equilibrium phases of the system obtained from Monte Carlo simulations are summarized in the phase diagram shown in figure 1. The phase diagram exhibits a phase in which the ordering corresponds to the AF states (region I), a phase in which the ordering corresponds to the AA states (region II) and a disordered phase (region III). The transition from the AF phase to the AA phase appears to be first order with clear discontinuities in M_{AF} and M_{AA} (figure 2). To the accuracy of the simulations, the value of J at which the transition between these two states occurs is independent of temperature. The phase boundary separating the ordered phases, AF (region I) and AA (region II), from the paramagnetic phase (region III) is obtained from the points at which the order parameters disappear (figure 3) and from the corresponding peak in the magnetic heat capacity (figure 4). Our simulations indicate that the transition is second order.

In addition we find evidence for two distinct AF phases. In one (AF1) the order parameter is parallel to one of the axes of the square lattice. In the other (AF2) the order parameter is at an angle of $\pi/4$ to the lattice axes. The existence of these two distinct phases is readily discerned by monitoring the angle associated with the sublattice magnetization for each of the four sublattices (see I for definitions and details). Figure 5 shows the behaviour of the sublattice magnetization angle as a function of decreasing temperature for three typical simulations. The dotted lines on the phase diagram indicate where a transition between the two AF phases is clearly observed in the simulations in region I for $T \lesssim 1.5g$. To the accuracy of the simulations, the value of J for each of these transitions is independent of temperature. For $T \gtrsim 1.5g$, the phase behaviour in region I becomes more difficult to determine and the phase boundary separating the two AF phases more difficult to discern. While it seems reasonable to suppose that the phase boundaries separating the two AF phases in region I remain distinct, terminating at the transition to the paramagnetic phase, at this point we cannot eliminate other possibilities. Despite these details regarding the precise determination of the phase boundaries

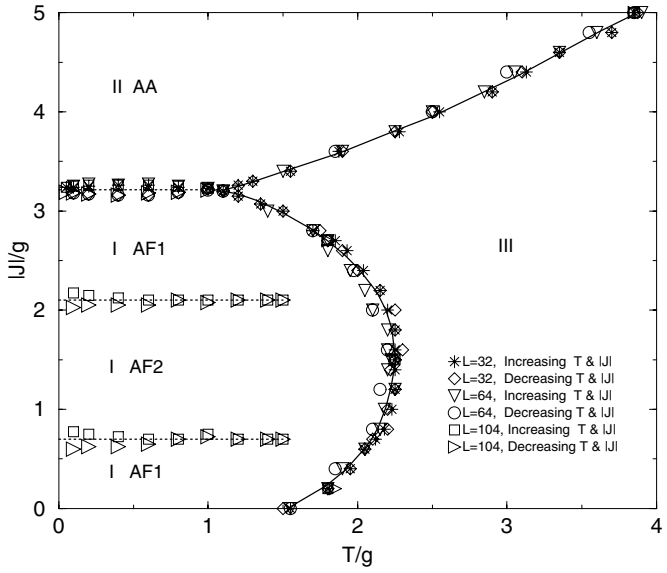

Figure 1. The phase diagram as a function of the exchange constant J and the temperature T.

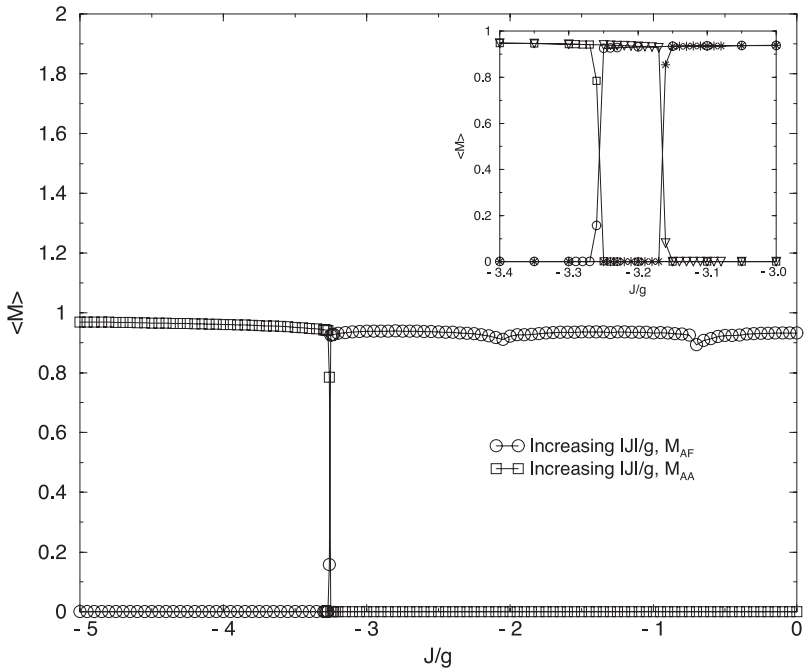

Figure 2. The order parameters M_{AF} and M_{AA} as a function of J for $T = 0.4g$. The transition region is shown in the inset and displays the hysteresis characteristic of a first-order transition.

separating the AF1 and AF2 phases, the reentrant behaviour of the AF phases, in which the system is in the AF1 phase for small values of $|J|$, switches to the AF2 phase as $|J|$ is increased and then back to the AF1 phase before the transition to the AA phase occurs, is perhaps the most remarkable feature of the phase diagram.

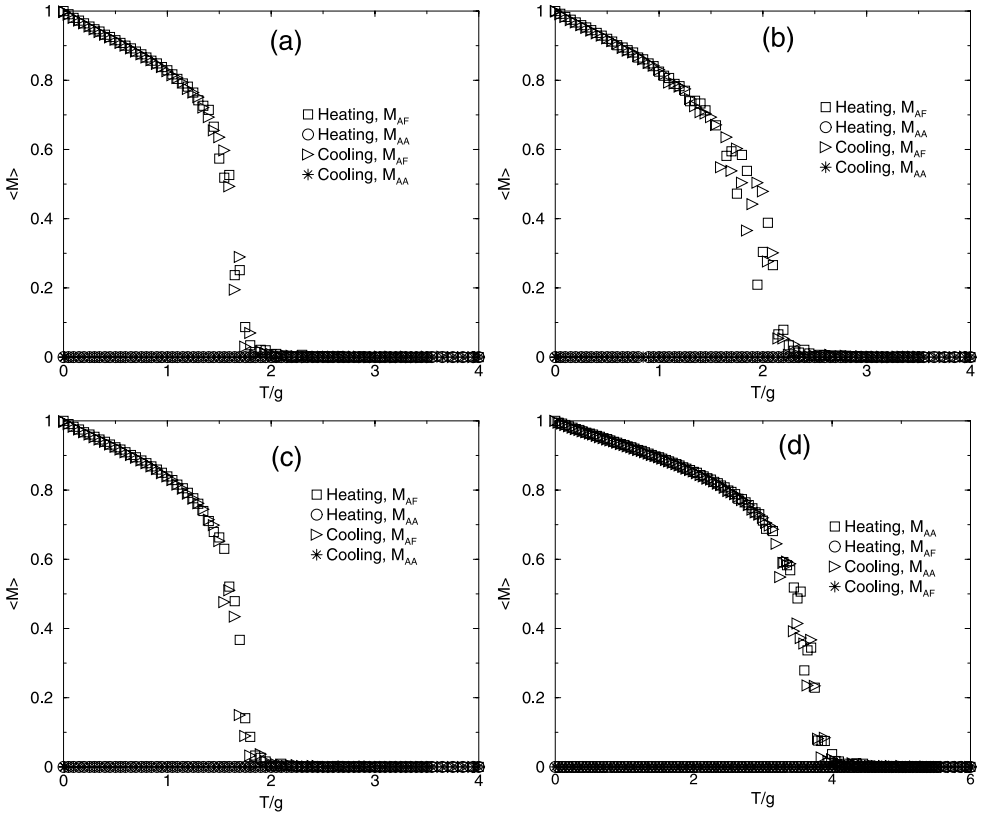

Figure 3. The order parameters M_{AF} and M_{AA} as a function of T for (a) $|J| = 0.2g$, (b) $|J| = 1.5g$, (c) $|J| = 2.7g$ and (d) $|J| = 5.0g$.

The two AF phases can also be distinguished by noting that the magnetic order in the AF phase arises as a consequence of an effective fourfold anisotropy induced by the thermal fluctuations which breaks the symmetry of the dipolar ground-state manifold [6, 8, 11]. The effect of this thermally induced effective anisotropy on the magnetic order can be determined by calculating the mean value of the conjugate field to which it couples [6], i.e.

$$P(T) = \frac{1}{N}\left\langle \sum_{\vec{R}} (\sigma_x^4 + \sigma_y^4) \right\rangle. \tag{5}$$

At zero temperature $P = 1$ for the AF1 phase and $P = 0.5$ for the AF2 phase, while in an isotropic phase $P = 0.75$. Figure 6 shows the variation of P with temperature for three values of J in the AF phases. In all three cases the data are for decreasing temperature. The graph shows two distinct behaviours. For $|J| = 0.2g$ and $2.7g$ the curve starts at high temperature in the paramagnetic phase with $P = 0.75$ and as the temperature is reduced P evolves towards a value of 1 in the limit $T \to 0$. For $|J| = 1.5g$ the behaviour is quite different: starting at high temperature in the paramagnetic phase, P decreases with decreasing temperature, reaching a value 0.5 in the limit $T \to 0$. This is consistent with the phase diagram shown in figure 1.

A noticeable feature of the curves for $|J| = 0.2g$ and $2.7g$ is that P reaches a value of 0.75, the expected value of P for an isotropic system, at $T \approx 1.4g$, just below the Néel temperature. A similar feature was noted in the analysis of the pure dipolar system [6]. The significance of this result and its implications for the magnetic order is not fully understood.

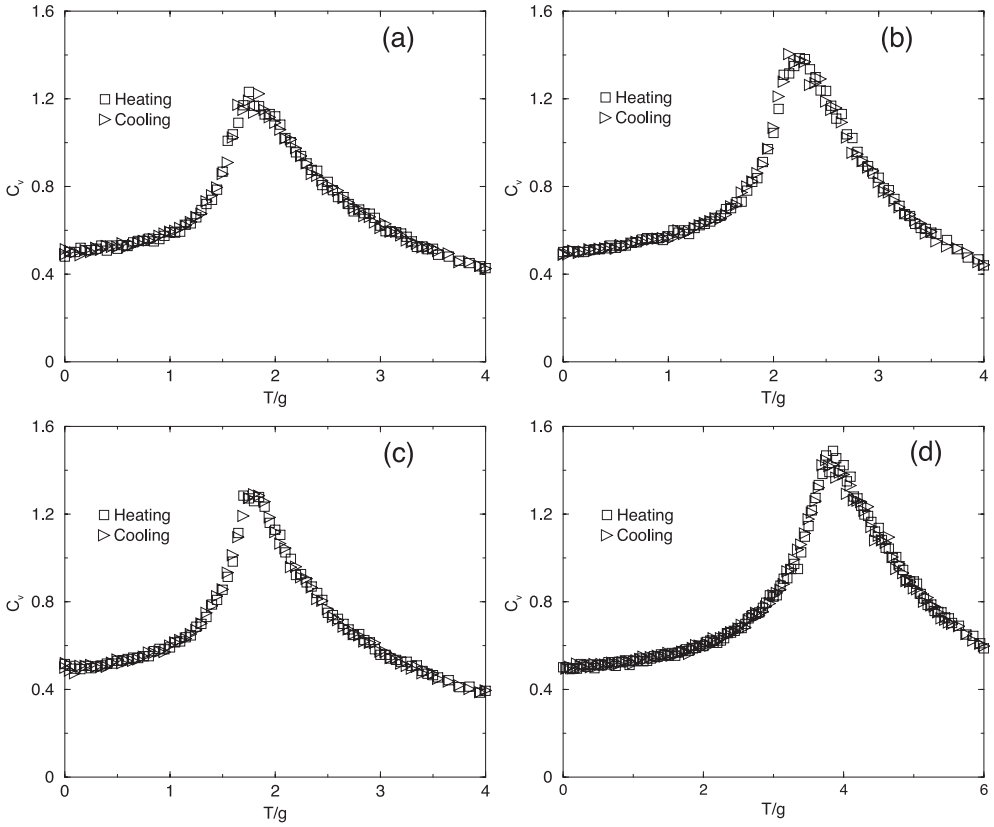

Figure 4. The heat capacity as a function of T for (a) $|J| = 0.2g$, (b) $|J| = 1.5g$, (c) $|J| = 2.7g$ and (d) $|J| = 5.0g$.

3. Free energy

The existence of the AF1 and the AF2 phases in region I of the phase diagram implies that the free energy in the AF phase has two branches, one branch corresponding to the AF1 phase and the other to the AF2 phase. The reentrant behaviour in which the antiferromagnetic AF phase changes not once but twice with increasing $|J|$ places constraints on the nature of the free energy surfaces describing the AF phases and how they intersect. It is therefore instructive to evaluate the free energy of the AF phase as a function of the exchange constant J for a fixed temperature T.

While the absolute free energy of a system cannot be calculated directly from simulations it is possible, using umbrella sampling techniques, to calculate the difference in free energy with respect to some reference state. It can be shown that the difference in free energy between two systems with different exchange constants can be expressed as

$$\Delta F(J) = F(J + \Delta J) - F(J) \tag{6}$$

$$= -T \log\left\langle \exp -\left(\Delta J \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j / T \right) \right\rangle_J \tag{7}$$

where the ensemble average is calculated with the exchange constant J. In practice reasonable results can be obtained from Monte Carlo simulations provided ΔJ is not too large. However,

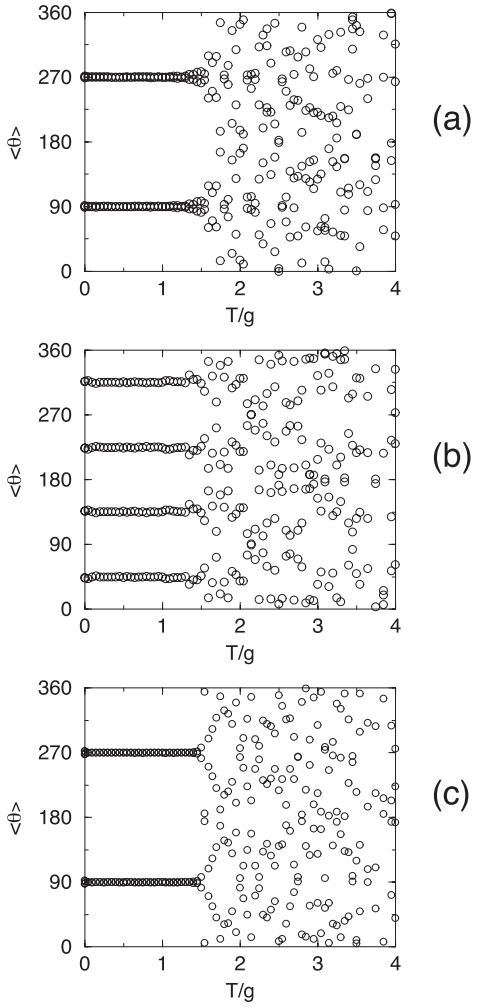

Figure 5. The angle of each of the four sublattice magnetizations as a function of decreasing temperature for (a) $|J| = 0.2g$, (b) $|J| = 1.5g$ and (c) $|J| = 2.7g$.

by calculating $\Delta F(J)$ for several values of J, the free energy can be calculated over a particular range of J using the fact that the free energy is a continuous function of J. Results are shown for $T = 0.2g$ in figure 7. The data shows that the free energy curves for both the AF1 and the AF2 phase are concave with a maximum around $|J| \approx 1.5g$ and are consistent with the reentrant behaviour obtained from the current simulations and implicit in the phase diagram shown in figure 1. Note however that the solid curves shown in figure 7 are simply a guide to the eye.

4. Conclusion

Returning to the question posed in the introduction, our present results demonstrate that a purely planar model can exhibit both the AF1 and AF2 phases with a transition between them as the relative strength of the exchange interaction is varied. Hence the out-of-plane degree

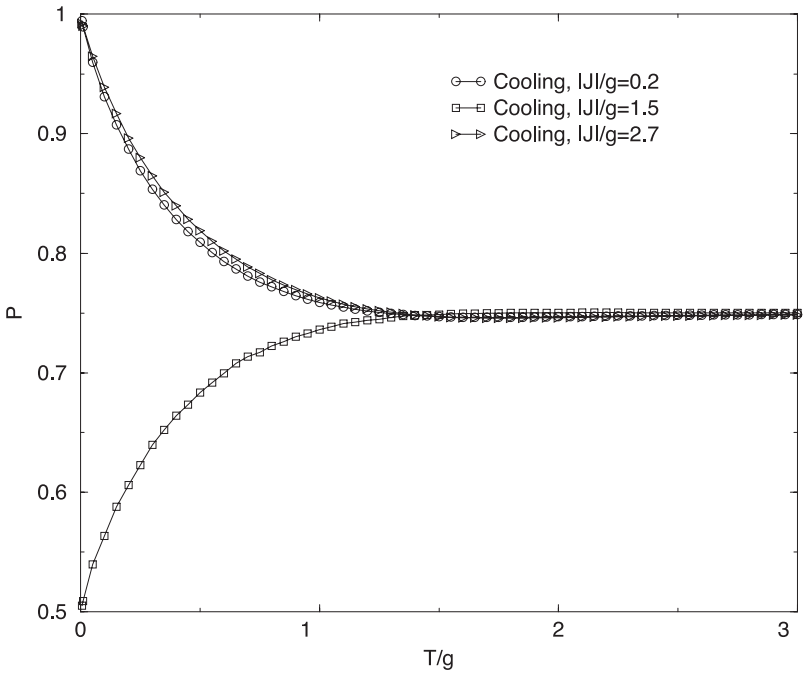

Figure 6. The conjugate field P as a function of decreasing T for several values of J.

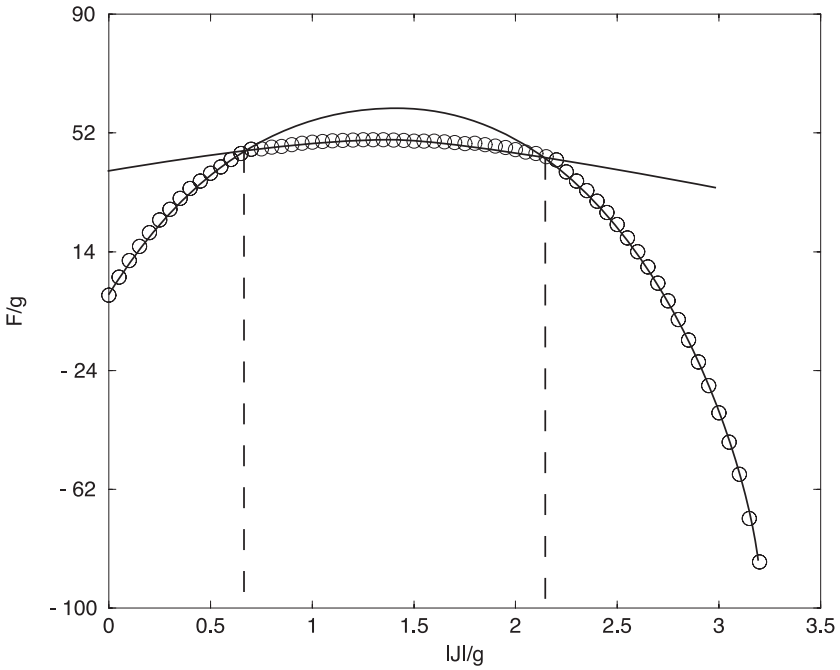

Figure 7. The free energy as a function of J for $T = 0.2g$. (The solid curves shown in the figure are simply a guide to the eye.)

of freedom of the magnetic moments, present in the study described in I but absent here, does not play a critical role in determining the easy axis of the magnetization in the AF phase. The question of how the presence of the exchange interaction modifies the thermal randomness so that this effect is observed remains to be answered. One approach that may provide some further insight into the role of the exchange interaction in the determination of the equilibrium phase would be to generalize the calculation of the free energy in the linearized spin wave approximation, presented in [6] for the pure dipolar case, to include the exchange interaction.

Further, our present study indicates that reentrant phenomena between the AF phases may occur as the relative strength of the exchange interaction is increased. This was not observed in the study reported in I, presumably because the in-plane to out-of-plane reorientation transition occurs before the system can reenter the AF1 phase. The low-temperature properties of the planar antiferromagnet therefore provide a particularly intriguing example of the phenomena of 'order from disorder'. It would be interesting therefore to examine how the antiferromagnetic order for the planar antiferromagnet would be affected by other types of disorder, such as dilution and quantum fluctuations; as the present work clearly demonstrates, the form of the ordered state is extremely sensitive to the precise nature of the disorder that gives rise to it.

Acknowledgments

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada. The authors gratefully acknowledge access to computational resources at The University of Calgary, provided under the auspices of C3.ca.

References

[1] De'Bell K, MacIsaac A B and Whitehead J P 2000 *Rev. Mod. Phys.* **72** 225
[2] 2000 *Economist* **18** 81
[3] Wolf S A, Awshalom D D, Buhrman R A, Daughton J M, von Molnár S, Roukes M L, Chtchelkanova A Y and Treger D M 2001 *Science* **294** 1488
[4] Venus D 1999 *Phys. Canada* September 267
[5] Abu-Labdeh A M, Whitehead J P, De'Bell K and MacIsaac A B 2002 *Phys. Rev.* B **65** 024434
[6] De'Bell K, MacIsaac A B, Booth I N and Whitehead J P 1997 *Phys. Rev.* B **55** 15 108
[7] Villain J, Bidaux R, Carton J P and Conte R 1980 *J. Physique* **41** 1263
[8] Henley C 1989 *Phys. Rev. Lett.* **62** 2056
[9] Henley C L 2001 *Can. J. Phys.* **79** 1307
[10] Bellier-Castella L, Gringas M J P, Holdsworth P C W and Moessner R 2001 *Can. J. Phys.* **79** 1365
[11] Prakash S and Henley C 1990 *Phys. Rev.* B **42** 6574