Phase diagrams of XY metamagnet

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Abstract: The three-dimensional XY model is considered in the presence of a uniform magnetic field applied in the X-direction. The nearest neighbour intraplanar interaction is considered ferromagnetic, and the interplanar nearest neighbour interaction is considered antiferromagnetic. Starting from a high-temperature initial random spin configuration, the equilibrium phase of the system at any finite temperature was achieved by cooling the system using the Monte Carlo single spin flip Metropolis algorithm with a random updating rule. The components of total magnetisation and the sublattice magnetisations were calculated. The variance of the antiferromagnetic order parameter and the specific heat were calculated. In a specific range of relative strengths of interactions (antiferromagnetic/ferromagnetic), the system shows multiple equilibrium phase transitions as observed from the double peaks of the specific heat plotted against the temperature. The phase diagrams (in the field-temperature plane) were obtained for different relative interaction strengths. The two boundaries meet at some bicritical point. As the strength of relative interaction increases, the bicritical point was found to move towards higher values of temperature and field.

Keywords: XY model, Monte Carlo simulation, Metropolis algorithm, Metamagnetic phases, Bicritical point
I. Introduction:

Magnetic field-induced phase transitions have been the focus of numerous theoretical and experimental works in condensed-matter physics and statistical physics over the last several decades. Metamagnetic systems under the influence of an external magnetic field can show unusual and interesting physical behaviours due to the competition between antiferromagnetic and ferromagnetic interactions. More specifically, the spins in the intralayer part of the system interact ferromagnetically with each other while they interact antiferromagnetically with each other along the interlayer part of the system. In the absence of an external field, a typical Ising metamagnetic system has an antiferromagnetic order. When the strength of the field is increased starting from zero, its phase transition point separating the ordered and disordered phases from each other gets shifted to the lower temperature region. From the theoretical point of view, thermal and magnetic phase transition properties of different kinds of metamagnetic systems have been studied by a wide variety of techniques such as Mean-Field Theory [1–8], Effective-Field Theory [9–13], Monte-Carlo simulation method [14–25], and High Temperature Series Expansion method [26, 27]. The studies done so far show us that metamagnetic systems can include multicritical points such as tricritical points, bicritical end points, and critical end points depending on the ratio between these ferromagnetic and antiferromagnetic interactions. As an interesting example, it is possible to say that the magnetic behaviour of a typical Ising antiferromagnet under the existence of a magnetic field is different from that found in $^3$He-$^4$He mixtures in the tricritical region [14]. In another work, Žukovic and Idogaki focused on the dilution effects on the multicritical behaviour observed in the metamagnetic systems by performing Monte Carlo simulations [22]. They reported that the region where a first order phase transition appears survived down to at least $p = 0.5$, where $p$ controls the density of the magnetic sites.

Furthermore, the metamagnetic systems can present multiple peaks in thermodynamic functions such as specific heat and susceptibility curves as a function of the temperature [17, 18, 20]. Readers may refer to [28] for a detailed review of the metamagnetism observed in many systems. We note that, among the many metamagnets, three of the most studied are $\text{FeBr}_2$, $\text{FeI}_2$ and $\text{FeCl}_2$. In addition to the equilibrium properties, many studies have been devoted to elucidating the nonequilibrium features of the metamagnetic systems driven by a time dependent magnetic field [29–32].

Most of these studies mentioned above are performed in discrete Ising type spin models. It is known that continuous classical spin models like $XY$ are of great interest because they have very rich physical behaviors. The order parameter belonging to the $XY$ model has only two components. For the first time, a new definition of order called topological order is proposed by Kosterlitz and Thouless for two-dimensional planar magnets like $XY$ ferromagnets in which no long-range ferromagnetic order exists [33]. Since then, magnetic properties of different kinds of systems have been handled with the $XY$ model. For instance, spin-dynamics regarding the structure factor and transport properties of the three-dimensional $XY$ model have been investigated by Monte-Carlo simulations [34]. Extensive Monte Carlo simulations of the classical $XY$ model in three dimensions containing random site dilution have been performed by using a hybrid algorithm [35]. Based on the numerical outcomes, it is found that the critical exponents and universal cumulants are independent of the amount of dilution. Recently, the $XY$ vectorial generalisation of the Blume-Emery-Griffiths model has been treated on thin films, and its thermodynamical properties are determined as a function of the film thickness [36]. It is shown that this model exhibits a very rich phase diagram, including Berezinskii-Kosterlitz-Thouless (BKT) transitions, BKT endpoints, and isolated critical points. By means of Monte Carlo simulations, surface critical behaviors,
including the corresponding critical exponents in the XY model, have been analysed in Ref. [37].

In the present study, we investigate the metamagnetic XY model on a three-dimensional lattice by benefiting from Monte Carlo simulation with local update. As far as we know, the thermal and magnetic phase transition properties of the model mentioned above have not been studied yet. In a nutshell, we show that the present system has very rich phase diagrams and exhibits multiple transitions depending on the competition between different kinds of spin-spin interactions.

The paper is organised as follows: In the next section (section II) the model and Monte Carlo simulation scheme are discussed. The numerical results are reported in section III. The paper ends with a summary of the work in section IV.

II. The Model and Simulation method:

The spin-1 XY metamagnet is modelled by the following Hamiltonian,

\[ H = -J_f \sum_{\text{intra-planar}} (S^x_i S^x_j + S^y_i S^y_j) - J_a \sum_{\text{inter-planar}} (S^x_i S^x_j + S^y_i S^y_j) - \sum_i (h_x S^x_i + h_y S^y_i), \]  

where \( S^x_i \) and \( S^y_i \) are the x and y-component of the spin \((S = 1)\) at \(i\)-th lattice site respectively. \((S^x_i)^2 + (S^y_i)^2 = 1\) always for all \(i\). \(J_f(>0)\) is nearest neighbour intra planar nearest neighbour ferromagnetic interaction strength and \(J_a(<0)\) is the nearest neighbour inter planar antiferromagnetic interaction strength. Here the ratio \((R)\) of the interaction strength is \(R = -\frac{J_a}{J_f}\). The \(h_x\) and \(h_y\) are the x and y components of the externally applied magnetic fields. Periodic boundary conditions are applied in all three directions.

In our simulation, we have considered \(L \times L \times L\) simple cubic lattice of \(L = 40\). The initial state of the system was considered with high temperature random configurations of spins. This is paramagnetic phase corresponding to a high temperature \((T)\) measured in the unit of \(J_f/k\), where \(k\) is Boltzmann constant. The system was updated by random updating scheme. In the random updating scheme, any lattice site (say \(i\)-th site) is chosen randomly where the old values of spin components \((S^x_i(\text{old}), S^y_i(\text{old}))\) have to be updated to another randomly chosen new values spin components \((S^x_i(\text{new}), S^y_i(\text{new}))\) according to the Metropolis probability

\[ P(S_{\text{old}} \rightarrow S_{\text{new}}) = \text{Min}[1, \exp(-\frac{\Delta H}{kT})] \]  

\(\Delta H\) is the change in energy due the change in spin configuration from old value to new value. If a random number (uniformly distributed between 0 and 1) is less than or equal to the Metropolis probability (mentioned above), then the randomly chosen lattice site will be assigned the new values of spin components. In this way, \(L^3\) such random updates are done. This constitutes a single Monte Carlo Step per Site (MCSS) and serves as the unit of time in this problem.

Throughout the simulation we have considered \(h_y = 0\) and allowed \(2 \times 10^5\) number of MCSS out of which we have discarded transient/initial \(1.5 \times 10^5\) number of MCSS. The observable quantities are measured/calculated by averaging over \(5 \times 10^4\) MCSS. We have checked that the initially discarded MCSS is sufficient to have equilibrium results within the accuracy of the interval of temperatures. In this way, just by cooling the system, from a high temperature paramagnetic phase, we have obtained various quantities as a function of temperature.
II. Results:

The present study is based on the proper characterization of various thermodynamic phases of the XY metamagnet. The different components of ferromagnetic and antiferromagnetic order parameters are responsible for representing the phases. The temperature at which the phase transition occurs can be determined by the thermal variations of the variance of different components of the order parameter (assumed to serve the role of susceptibility) and the specific heat. Keeping this in mind, we have calculated the following quantities:

(1) X-component of the antiferromagnetic order parameter \(M^x_a\):

\[
m^x_a = \frac{1}{L^3} \left( \sum_{\text{odd planes}} S^x_i - \sum_{\text{even planes}} S^x_i \right)
\]

\[
M^x_a = \langle m^x_a \rangle = \frac{1}{\tau} \int m^x_a dt
\]

(2) Y-component of the antiferromagnetic order parameter \(M^y_a\):

\[
m^y_a = \frac{1}{L^3} \left( \sum_{\text{odd planes}} S^y_i - \sum_{\text{even planes}} S^y_i \right)
\]

\[
M^y_a = \langle m^y_a \rangle = \frac{1}{\tau} \int m^y_a dt
\]

(3) X-component of ferromagnetic ordering \(M^x_f\):

\[
m^x_f = \frac{1}{L^3} \left( \sum_{\text{odd planes}} S^x_i + \sum_{\text{even planes}} S^x_i \right)
\]

\[
M^x_f = \langle m^x_f \rangle = \frac{1}{\tau} \int m^x_f dt
\]

(4) Variance of antiferromagnetic Y-ordering:

\[
\chi_{ay} = \left| m^y_a \right|^2 - \left( \langle m^y_a \rangle \right)^2
\]

(5) Mean angle (odd plane) \(\theta_o\):

\[
\theta_o = \frac{2}{\sqrt{3}} \sum_{\text{Odd planes}} \tan^{-1} \left( \frac{S^y}{S^x} \right)
\]

(6) Mean angle (even plane) \(\theta_e\):

\[
\theta_e = \frac{2}{\sqrt{3}} \sum_{\text{Even planes}} \tan^{-1} \left( \frac{S^y}{S^x} \right)
\]

(7) Specific heat \(C\):

\[
\frac{dE}{dT} \approx \frac{E(T+\Delta T) - E(T-\Delta T)}{2\Delta T}
\]

\[
C = \frac{dE}{dT} \approx \frac{E(T+\Delta T) - E(T-\Delta T)}{2\Delta T}
\]

The above mentioned thermodynamic quantities are studied as functions of temperature, as shown in the figures. Figure 1 shows the thermal variations of different order parameters. As the temperature of the system decreases (for \(R = 0.4\) and \(h_x = 0.8\)), the antiferromagnetic ordering in the Y-direction \(M^y_a\) was found to take a nonzero value (Fig 1(a)) at some transition temperature \(T_c\), whereas the antiferromagnetic ordering along the X-direction \(M^x_a\) remains zero for all temperatures. The ferromagnetic ordering in the X-direction \(M^x_f\) assumes a nonzero value due to the application of an external magnetic field \(h_x\) in the X-direction. A significant value of the maximum of \(M^x_f\) has been observed near the transition point. This transition point was found to shift towards the low temperature for a larger value of the \(h_x\) (Fig 1(b)).

The configurations of the spins are studied for different sublattices (denoted by odd numbered planes and even numbered planes). A typical such spin configuration is shown in Fig 2. The spin configuration in the low temperature ordered phase, shows that the values of \(M^y_a\) is nonzero in the ordered phase. The value of \(M^x_a\) remains zero for the entire range of the temperature, whereas the nonzero value of \(M^x_f\) is also evident. In the high temperature intermediate phase, the antiferromagnetic ordering is dominated by the ferromagnetic ordering in the X-direction. The intermediate phase is not completely random, where no (ferromagnetic/antiferromagnetic) ordering is present.
The transition temperature for the different values of $h_x$ can also be determined from the temperature dependences of $\chi_{ay}$ (the variance of $M_y$). The $\chi_{ay}$ are plotted against temperature for two different values of $h_x$ and shown in Fig.3. The temperature which maximizes $\chi_{ay}$ is indicating the transition (from paramagnetic to antiferromagnetic ordering in Y-direction) temperature. For lower values of $h_x$ the system shows a single phase transition, but for higher values of $h_x$ it shows a double phase transition. This feature is not evident from the study of $\chi_{ay}$ as a function of temperature, since it shows only one peak for all values of the field $h_x$.

The double phase transitions, for larger values of the field $h_x$, has been observed from the study of specific heat $C$ as function of the temperature $T$. This is shown in Fig.4 For lower values of $h_x(= 0.8)$ the specific heat $C$ gets peaked at one temperature only (Fig.4(a)). However, for a higher value of $h_x(= 1.2)$, two distinct peaks are observed (Fig.4(b)). Apart from the low temperature antiferromagnetic (in Y-direction) phase, another intermediate phase has been observed, in the temperature range, between the positions of the two peaks of the specific heat (for higher values of $h_x$).

For this particular reason, we have plotted the comprehensive phase boundary ($T_c$ as function of $h_x$) just by collecting the values of temperature for which $C$ has maxima. The phase boundary for $R = 0.2$ has been shown in Fig.5 Here two boundaries meet at a particular point (the bicritical point) and are shown by a big open circle in the phase diagram.

The shape of the phase diagram is qualitatively similar for different values of $R$. The phase diagrams for $R = 0.4$ (Fig.6) and $R = 0.6$ (Fig.7) are shown. The bicritical point was found to shift towards higher temperatures and higher values of $h_x$ as the value of $R$ increased.

The low field para-antiferro transition can also be observed by studying the mean angle of two sublattices ($\theta_e$ for even numbered planes and $\theta_o$ for odd numbered planes). In the paramagnetic phase, the mean sublattice angles are the same and approximately equal to $\pi$. But below the critical temperature, the mean angles of different sublattices get widely apart, confirming the antiferromagnetic ordering in the Y-direction. These are shown in Fig.8.

We have investigated the effects of different values of $R$ in the specific heat as a function of temperature. The antiferromagnetic phase transition is observed (as shown in the Fig.9) to occur at a high temperature for higher values of $R$.

For various system sizes, the susceptibility of $\chi_{ay}$ as a function of temperature, is investigated. Here, we have considered, $L = 20, 30$ and $40$. The results are shown in Fig.10. The height of the peak of susceptibility increases for larger systems. This is an indication of the growth of correlation, which establishes the usual behaviour of critical phenomena.

IV. Summary:

We have done an MC simulation of a cubic lattice of size $L=40$. Initially, 150000 MCSS were discarded and the average was calculated over the next 50000 MCSS. The total length of the simulation is 200000 MCSS. Random updates of $L^3$ spins are considered a single MCSS.

Depending on the value of $h_x$ and $R$ the system undergoes equilibrium phase transitions. The antiferromagnetic ordering along the Y-direction grows at a critical temperature, which is obtained from the position of the peak of susceptibility, $\chi_{ay}$. For lower values (0.8 say) of the field $h_x$ ($h_y=0$ in these simulations), a single transition was observed. However, for higher values (say 1.2) the specific heat shows two peaks, indicating two transitions. For higher values of $h_x$, an intermediate
phase was observed in the temperature range between the two peaks of the specific heat. The two phase boundaries meet at a bicritical point in all the phase diagrams for $R = 0.2$, $R = 0.4$ and $R = 0.6$. As $R$ increased, the bicritical point was observed to shift towards higher temperatures and higher field values.

The mean sublattice angles of spin (measured from the positive x-axis) for odd and even planes are plotted against temperature and shown. The existence of a low-temperature antiferromagnetic phase was also found from the variations of mean sublattice angles with respect to temperature.

The configurations of spins are shown in Fig[2]. Here, the spin configurations for two consecutive (8th and 9th) planes are shown in two different ($T=0.5$ and $T=1.25$) temperatures. The high temperature spin configuration shows the ferromagnetically (in X-direction) dominated phase and the low temperature antiferromagnetically (in Y-direction) dominated phase.

The growth of the correlation was indeed observed near the transition temperature. The height of the peak susceptibility increases as the size of the system increases. It is believed that the susceptibility eventually diverges at the thermodynamic limit.

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Figure 1: The various ordering versus temperature.
Figure 2: The configurations of spin in the low temperature antiferromagnetic phase and in the high temperature intermediate phase. The two colours represent two planes (8th and 9th plane).
Figure 3: The Variance of $M^y_{a}$ versus temperature.
Figure 4: The Specific heat versus temperature.
Figure 5: The comprehensive phase diagram for $R=0.2$. 
Figure 6: The comprehensive phase diagram for R=0.4. The symbol 'O' represents the imaginary location of bicritical point.
Figure 7: The comprehensive phase diagram for R=0.6. The symbol 'O' represents the imaginary location of bicritical point.
Figure 8: The average angles of odd ($\theta_o$) and even ($\theta_e$) planes for R=0.4 for two different values of $h_x$. 
Figure 9: The specific heat ($C$) plotted against the temperature ($T$) for different values of $R(=0.4, 0.6, 0.8, 1.0, 1.2, 1.4)$. The value of $h_x = 1.0$ in all cases.
Figure 10: $\chi_{ag}$ versus temperature for different system sizes.