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Numerical solution of the mean-field theory of the ANNNI model in an external field: a comparison of two methods

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Abstract. It is shown how the solution of the mean-field equations for the ANNNI model can be reduced to the iteration of an area-preserving two-dimensional mapping if an external magnetic field is applied. This method is analysed in detail and compared with the exact numerical solution of the mean-field equations for simple periodic magnetisations.

1. Introduction

Since the discovery of spatially modulated phases in several magnetic materials (Habenschuss *et al* 1974, Rossat-Mignod *et al* 1980) simple theoretical models which lead to a better understanding of modulated phases have been studied intensively. These models, for example the axial next-nearest-neighbour Ising or ANNNI model (Elliot 1961, Hornreich *et al* 1979, Selke and Fisher 1979, 1980, Fisher and Selke 1980, Selke 1981, Rujan 1981, Williams *et al* 1981, Barber and Duxbury 1981, 1982) and the chiral Potts or asymmetric clock model (Ostlund 1981, Huse 1981), have been investigated by a variety of different methods. The topology of the phase diagram has been studied very successfully by the mean-field theory (MFT) of these models (Bak and Boehm 1980, Yokoi *et al* 1981, Öttinger 1983).

However, the mean-field equations are not exactly solvable even for models which have a spatially modulated magnetisation along one axis only and a constant magnetisation perpendicular to this axis. In this paper two methods of solving approximately the MFT or the ANNNI model on a cubic lattice in the presence of an external magnetic field are compared. These methods are as follows.

(1) Assuming a periodic magnetisation the mean-field equations can be solved numerically on small finite lattices (Bak and Boehm 1980, Yokoi *et al* 1981).

(2) Approximate solutions of the mean-field equations can be generated by iterating an area-preserving two-dimensional mapping (Bak 1981).

In the following, the first method will be called the 'simple commensurate method' (SCM) and the second method will be called the 'iterated mapping method' (IMM).

A further goal of this paper is to show how the MFT of the ANNNI model can be treated by the IMM if an external magnetic field is applied.

In the next section the MFT of the ANNNI model and the two methods of solving it numerically are described. The results of these methods will be compared in the third section. A brief summary concludes the paper.

2. MFT of the ANNNI model

The ANNNI model is an Ising model with competing ferromagnetic nearest-neighbour ($J_1 > 0$) and antiferromagnetic next-nearest-neighbour interactions ($J_2 < 0$) along one axis. Perpendicular to this axis there is only a ferromagnetic interaction ($J_0 > 0$) between nearest neighbours. Assuming the ferromagnetic coupling J_0 to produce layers of constant magnetisation, the mean-field free energy per site of the three-dimensional ANNNI model in an external field h is, apart from a constant term, (Yokoi *et al* 1981)

$$F = -(2N)^{-1} \sum_z M_z [4J_0 M_z + J_1(M_{z-1} + M_{z+1}) + J_2(M_{z-2} + M_{z+2})] - (h/N) \sum_z M_z + (k_B T/2N) \sum_z [(1+M_z)\ln(1+M_z) + (1-M_z)\ln(1-M_z)] \tag{1}$$

where M_z is the average magnetisation of the zth layer and N is the number of layers. The average magnetisations M_z are found by minimising the free energy.

The SCM is based on the numerical solution of the mean-field equations

$$M_z = \tanh\{(k_B T)^{-1}[4J_0 M_z + J_1(M_{z-1} + M_{z+1}) + J_2(M_{z-2} + M_{z+2}) + h]\} \tag{2}$$

which characterise the magnetisations for which the free energy (1) is stationary. In order to solve these equations it is assumed that M_z is periodic with period N ($N \leqslant 18$ in this paper). By this assumption the infinite system of equations (2) is reduced to a system of N equations which, in general, allow many solutions. The physical solution minimises the free energy (Bak and Boehm 1980, Yokoi *et al* 1981).

The drawback of the SCM is that by assuming periodic solutions with small periods only a few wavenumbers can occur. Therefore, only simple commensurate phases can be found; higher commensurate and incommensurate phases are excluded. This drawback is avoided if the free energy is minimised by the IMM.

The IMM is based on the ansatz

$$M_z = m + A\cos[2\pi(\tfrac{1}{4}z) + \phi_z] \tag{3}$$

where m is influenced by the external field h. $\phi_z = \frac{1}{4}\pi$ = constant describes the $q = \frac{1}{4}$ commensurate phase, $\phi_z = wz$ is a phase with $q = \frac{1}{4}[1 + (2w/\pi)]$. Using $\phi_{z+2} - 2\phi_{z+1} + \phi_z \ll 2(\phi_{z+1} - \phi_z) \ll 1$ for wavenumbers near $q = \frac{1}{4}$ and with the ansatz (3) the free energy (1) can be written as (apart from constants and terms that cancel on summing over the lattice)

$$F = \frac{2|J_2|A^2}{N} \sum_z [\tfrac{1}{2}(\phi_{z+1} - \phi_z + \delta)^2 + aV_{mA}(\phi_z)] \tag{4}$$

where J_1 and J_2 are parametrised by a and δ:

$$J_1 = 8\delta a A^2 k_B T \qquad J_2 = -2aA^2 k_B T. \tag{5}$$

The potential $V_{mA}(\phi)$ which generalises the case $m = 0$ (Bak 1981) is

$$V_{mA}(\phi) = \tfrac{1}{4}(I(m + A\cos\phi) + I(m - A\cos\phi) + I(m + A\sin\phi) + I(m - A\sin\phi)), \tag{6a}$$

where

$$I(x) = \int_0^x \tanh^{-1}\sigma \, d\sigma = \tfrac{1}{2}[(1+x)\ln(1+x) + (1-x)\ln(1-x)]. \tag{6b}$$

The physical phases ϕ_z minimise the free energy (4). F is stationary if

$$w_{z+1} = w_z + a V'_{mA}(\phi_z) \tag{7a}$$

where w_{z+1} is defined by

$$\phi_{z+1} = \phi_z + w_{z+1}. \tag{7b}$$

These equations define an area-preserving two-dimensional iterated mapping, the trajectories of which (independent of δ, this is independent of J_2/J_1) determine the magnetisation for which F is stationary (via equation (3)). Without any difficulty the magnetisation along the axis with competing interactions can be calculated for several thousand sites. For each δ the trajectory which yields the minimum of the free energy has to be found.

The drawback of the IMM is the indirect definition of J_0 and h by A and m (J_1 and J_2 can be varied directly by varying a and δ). In order to determine J_0 and h one can plot

$$f(M_z) = k_B T \tanh^{-1} M_z - J_1(M_{z-1} + M_{z+1}) - J_2(M_{z-2} + M_{z+2}) \tag{8}$$

against M_z for the trajectory which minimises F. The validity of the approximations leading to equation (4) can be estimated by the deviation of $f(M_z)$ from a straight line, because according to equation (2) $f(M_z) = 4J_0 M_z + h$. J_0 and h can be determined by fitting a straight line to $f(M_z)$.

3. Numerical results

Figure 1 shows the results of computer iterations of equations (7) for $A = 0.71$, $a = 3.68$ and $m = 0.1$ (1500 iterations for each trajectory). The figure is very similar to the

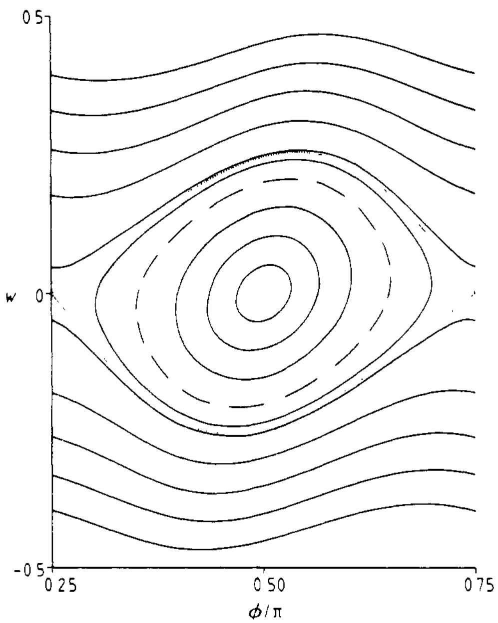

Figure 1. Trajectories of the iterated mapping (7). $A = 0.71$, $a = 3.68$ and $m = 0.1$.

corresponding figure for $m = 0$ (Bak 1981), but with increasing m the central bubble becomes larger. The fixed point $\phi_z = \frac{1}{4}\pi$ (or equivalently $\phi_z = \frac{3}{4}\pi$), $w_z = 0$ describes the previously mentioned $q = \frac{1}{4}$ phase, the fixed point $\phi_z = \frac{1}{2}\pi$, $w_z = 0$ corresponds to the magnetisation $m, m - A, m, m + A \ldots$ along the axis and is always unstable (maximum of the free energy). The closed orbits around this fixed point describing the same commensurate phase with an incommensurate modulation are also always unstable.

The smooth invariant trajectories below the central bubble are stable for appropriate values of δ. For these trajectories the mean value of w_z is $\bar{w} < 0$ and thus $q = \frac{1}{4}[1 + (2\bar{w}/\pi)] < \frac{1}{4}$. Taking into account the fluctuations of w_z around $\bar{w}$, ϕ_z can be written in a form characteristic for incommensurate phases:

$$\phi_z = (\bar{w}z + \alpha) + g(\bar{w}z + \alpha) \tag{9}$$

where g is a periodic function with period $\frac{1}{2}\pi$ and α is an arbitrary phase.

Figure 2 shows a plot of the wavenumbers obtained from the stable trajectories against δ. For each value of δ the free energies of some 1000 trajectories were computed (1500 iterations for each trajectory). For comparison the step function $q(\delta)$ obtained by the SCM on lattices of length $N \leqslant 18$ is also shown. In order to apply the SCM, $f(M_z)$ (equation (8)) was plotted against M_z (figure 3 for example) and the parameters J_0 and h for which the mean-field equations $f(M_z) = 4J_0M_z + h$ are solved optimally were obtained by linear regression (J_1 and J_2 are defined by (5)). The small deviation of $f(M_z)$ from a straight line justifies the approximations used in the IMM.

For a further check the mean values of the magnetisations obtained by the SCM were computed. The deviations from the IMM value $M = 0.1$ are less than five per cent for $\delta < 0.27$ and less than ten per cent for larger values of δ. The IMM shows no 'lock-in' of simple commensurate wavenumbers for the parameters considered so far. The results of the SCM are, therefore, quite misleading.

Figure 4 shows the results of computer iterations of equations (7) for $A = 0.71$, $\alpha = 8$ and $m = 0.1$. For these parameters, corresponding to a lower temperature and a weaker magnetic field, chaotic trajectories and small bubbles between the smooth invariant trajectories can be observed. These small bubbles are miniature reproductions of figure 1. The corresponding trajectories jump from bubble to bubble. Again

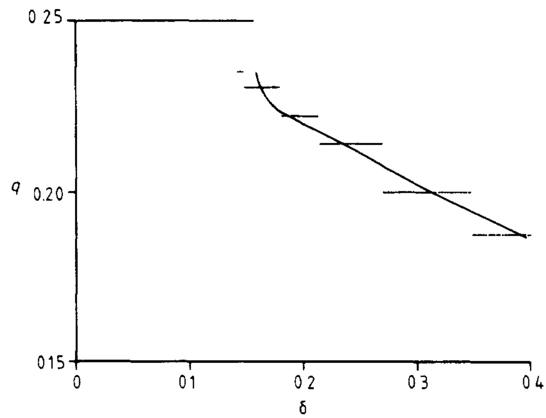

Figure 2. Wavenumber q against $\delta = -(J_1/4J_2)$ for $A = 0.71$, $a = 3.68$ and $m = 0.1$.

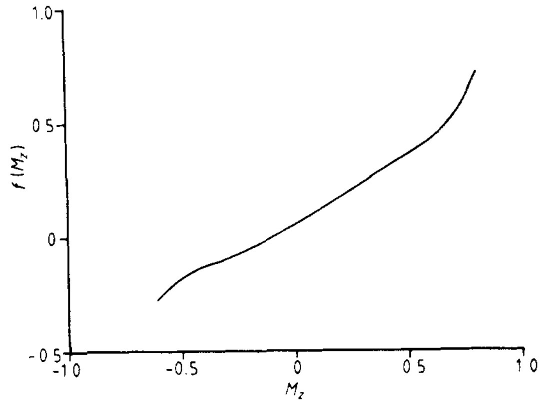

Figure 3. $f(M_z)$ against M_z for $A = 0.71$, $a = 3.68$, $m = 0.1$ and $\delta = 0.2$.

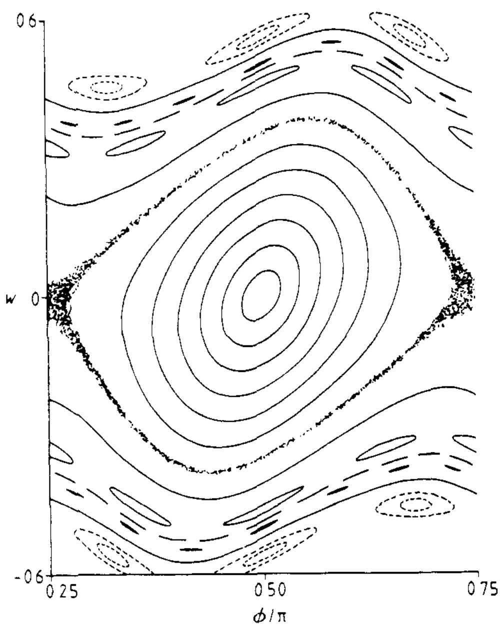

Figure 4. Trajectories of the iterated mapping (7). $A = 0.71$, $a = 8$ and $m = 0.1$.

the trajectories within the bubbles are always unstable and the points between the bubbles which form a limit cycle with a few points only (fixed point for the central bubble) describe stable commensurate phases. For instance the four points, between the four bubbles below the central bubble, correspond to a wavenumber $q = \frac{1}{4}(1 - \frac{1}{4}) = \frac{3}{16}$. Trajectories yielding wavenumbers $\frac{2}{9}$, $\frac{7}{32}$, $\frac{3}{14}$, $\frac{11}{52}$, $\frac{5}{24}$, $\frac{9}{44}$, $\frac{1}{5}$, $\frac{7}{36}$, $\frac{3}{16}$, $\frac{2}{11}$, $\frac{5}{28}$ and $\frac{7}{40}$ have been found. Figure 5 shows the wavenumbers that lock-in at certain values of δ. The computations have been done with a step width of $\frac{1}{1000}$ for δ and some 2500 trajectories.

Figure 6 shows the good agreement of the magnetisations obtained by the IMM and the SCM in the $q = \frac{2}{9}$ phase. The wavenumbers $\frac{1}{4}$, $\frac{2}{9}$, $\frac{1}{5}$ and $\frac{3}{16}$ obtained by the IMM

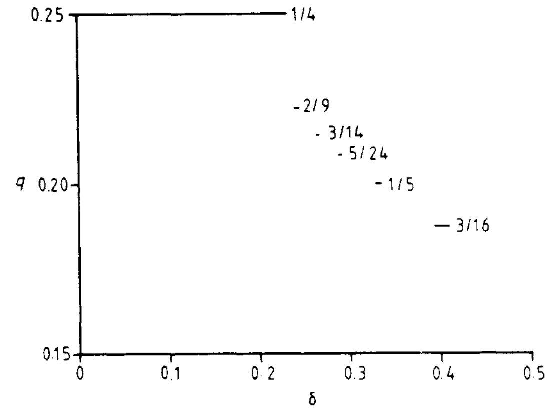

Figure 5. Simple commensurate wavenumbers obtained by the IMM for $A = 0.71$, $a = 8$ and $m = 0.1$.

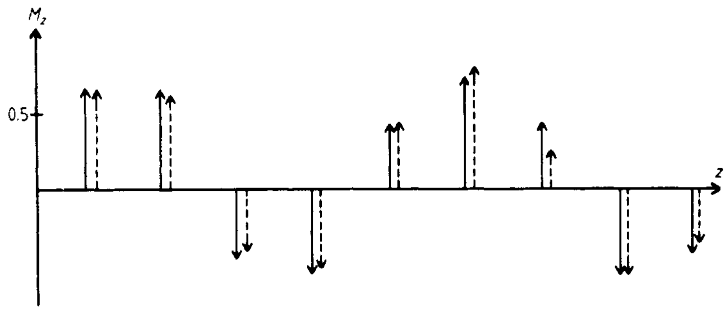

Figure 6. Comparison of the magnetisations along the axis with competing interactions for the $q = \frac{2}{9}$ phase ($A = 0.71$, $a = 8$, $m = 0.1$ and $\delta = 0.24$). Broken arrows, IMM; full arrows, SCM.

are also found by the SCM. In order to avoid large deviations from the IMM mean magnetisation $m = 0.1$ being favoured by the SCM, the magnetisations M_z in the magnetic term of the free energy (1) were replaced by the IMM value m (the SCM yields $m = 0.134$ in the $q = \frac{3}{16}$ phase and $m = 0.150$ in the $q = \frac{1}{5}$ phase). The IMM wavenumbers $\frac{3}{14}$ and $\frac{5}{24}$ are merely metastable because the free energy obtained by the SCM is slightly smaller for the wavenumbers $\frac{2}{9}$ and $\frac{1}{5}$ respectively. The IMM yields simple commensurate phases, although using the IMM there is, in contrast to the SCM, no necessity for these phases to occur. A second new feature figure 4 shows, as compared with figure 1, are the chaotic trajectories surrounding the central bubble (around the small bubbles and in figure 1 such trajectories also exist). These trajectories stay near the fixed point $\phi_z = \frac{3}{4}\pi$, $w_z = 0$ ($q = \frac{1}{4}$ phase) for many iterations (lattice sites) and after some time, which is random, they jump in a few iterations to the equivalent fixed point $\phi_z = \frac{1}{4}\pi$, $w_z = 0$, where they stay again for many iterations ($q = \frac{1}{4}$ phase). Therefore, chaotic trajectories correspond to commensurate phases with local perturbations, 'solitons', that slightly alter the wavenumber. These phases were conjectured to be stable by Bak (1981). This conjecture is incorrect; the chaotic trajectories correspond at most to metastable configurations (Aubry 1982).

4. Summary

In this paper the MFT of the three-dimensional ANNNI model in an external field was studied by two different methods. Using the uncomplicated SCM, the exact numerical solution of the mean-field equations for simple periodic magnetisations, a 'lock-in' of commensurate phases cannot be demonstrated significantly because only a few simple wavenumbers can occur in this method.

The more laborious IMM, which reduces the solution of the MFT to the iteration of an area-preserving two-dimensional mapping, corresponds to the approximate solution of the mean-field equations on huge lattices, thus admitting arbitrary wavenumbers. Besides the commensurate phases of the SCM, incommensurate phases and commensurate phases with localised perturbations ('solitons randomly pinned to the lattice') can be found by the IMM.

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