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Phase transitions in quasi-periodic superlattices

Jian Yuan
Institute of Physics, Academia Sinica, Beijing, People's Republic of China

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Abstract. We investigate numerically the magnetic-field- and temperature-dependent equilibrium structure of finite quasi-periodic superlattices formed from two kinds of magnetic films arranged in the Fibonacci way. Different kinds of equilibrium structures are obtained. It is shown that small changes in the quasi-periodic structures can lead to dramatic changes in the H–T phase diagrams.

1. Introduction

A number of recent papers have studied phase transitions in antiferromagnetic superlattice structures [1, 2], in which some of the constructing films couple antiferromagnetically. Some interesting magnetic properties of these materials have been found. For example, in a superlattice composed of ferromagnetic films alternating with antiferromagnetic films, the ground state of the system is found to depend on whether the number of atomic planes in each antiferromagnetic film is even or odd [1]. We note that the above-mentioned superlattice structures are periodic structures in which the two kinds of constructing films are alternated periodically. Recently, new kinds of superlattice structures, quasi-periodic superlattices, have appeared in the laboratory [3]. In these new structures, periodicity no longer exists in the direction perpendicular to the constructing films in the strict sense. Many new unusual phenomena have been found in such new structures [4]. In this paper, we start to investigate the magnetic-field- and temperature-dependent equilibrium structure of these quasiperiodic superlattices formed from magnetic films.

2. Model and calculation method

Quasi-periodic structures may be constructed by two kinds of blocks A and B, arranged according to the Fibonacci sequence S_q, which satisfies the recursive relation $S_{q+1} = \{S_q, S_{q-1}\}$ for $q \geqslant 1$ with $S_0 = \{B\}$ and $S_1 = \{A\}$. The first few sequences are as follows:

$$S_2 = AB$$

$$S_3 = ABA$$

$$S_4 = ABAAB$$

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$$S_5 = ABAABABA$$

. . . .

If we replace each block A and B in sequence S_q by two kinds of magnetic films, say Gd and Fe films, respectively, and assume the number of microscopic layers inside film Gd(Fe) is l_{Gd} (l_{Fe}), then we obtain a finite quasi-periodic superlattice. In the following, we will discuss the phase transitions in this finite quasi-periodic superlattice in the presence of an external field H_0 applied in the direction x parallel to the films.

For simplicity, we neglect the anisotropy field in Gd and assume the Gd and Fe films have the same structure (BCC structure) [2] but with different spins ($s = \frac{7}{2}$ and $\frac{5}{2}$ respectively). In this system, the Fe and Gd spins are free to rotate in the film planes (the spins are not likely to have static components in the direction perpendicular to the films because this would set up static demagnetising fields [2]). The exchange coupling constant between Gd spins is J_1, that between Fe spins in J_2 and that between a Gd and a Fe spin is J_I. Here only the nearest-neighbour interactions are considered, the inclusion of additional neighbours is straightforward [2]. In this work these parameters have the values $J = 0.155$, $J_2 = 1$ and $J_I = -1$, since experimental results [5, 6] show that the interface coupling between Gd and Fe is antiferromagnetic even though both materials are ferromagnetic in the bulk. The boundary condition we take in this work is the 'free surface' condition, where the interaction across the surface of the finite system is set to zero, which is a good approximation to the actual case when the substrate of the superlattice made in the laboratory is formed from non-magnetic materials†.

For a given temperature T and an applied field H_0, the magnetic state of the system can be described by a set of $\{\theta_j\}$ which give the orientation of the spins in the films with respect to the x axis and a set of $\{\langle s_j\rangle\}$ which give the thermal averaged magnitude of the spins in the films. The purpose of our numerical calculations is to find out the state which is a stable state with the lowest free energy for the system at the given T and H_0. In order to do that, similarly to [2], we first choose an initial configuration of $\{\theta_j\}$ and a set of initial values of $\{\langle s_j\rangle\}$, then we randomly pick a spin in a particular layer j and rotate the spin s_j into the direction of the effective field, which is given by the following equation for the present system:

$$H_j = 4(J_{j,j+1}\langle s_{j+1}\rangle \boldsymbol{r}_{j+1} + J_{j,j-1}\langle s_{j-1}\rangle \boldsymbol{r}_{j-1}) + H_0 \boldsymbol{x}$$

where $J_{j,j+1}$ is the exchange coupling constant between layers j and $j+1$ and $\boldsymbol{r}_j$ is the unit vector in the previous direction of the spin s_j. The thermal averaged magnitude of the spin s_j in the new direction is now:

$$\langle s_j\rangle = s_j B_{s_j}(x)$$

where

$$x = s_j H_j / k_B T$$

and the Brillouin function is given by:

$$B_s(x) = \frac{2s+1}{2s}\coth\left(\frac{2s+1}{2s}x\right) - \frac{1}{2s}\coth\left(\frac{x}{2s}\right).$$

We repeat this operation step by step for all spins until a self-consistent state is obtained,

† If we take periodic instead of 'free surface' boundary conditions and consider the next-nearest-neighbour interactions, the phase diagrams obtained in this work may be more complicated, since there may exist some (long-period) commensurate phases. References on related problems can be found in a review article by Bak [7].

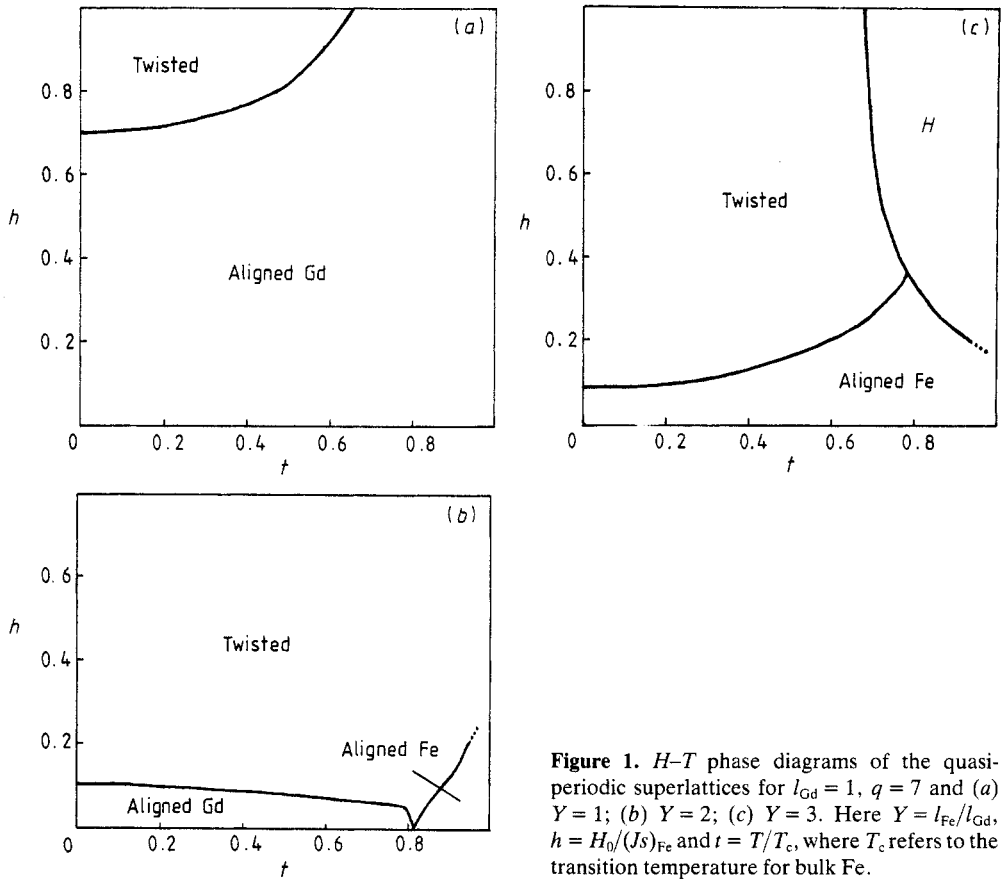

Figure 1. H–T phase diagrams of the quasi-periodic superlattices for $l_{Gd} = 1$, $q = 7$ and (*a*) $Y = 1$; (*b*) $Y = 2$; (*c*) $Y = 3$. Here $Y = l_{Fe}/l_{Gd}$, $h = H_0/(Js)_{Fe}$ and $t = T/T_c$, where T_c refers to the transition temperature for bulk Fe.

the only interesting state at present is the stable state with the lowest free energy, which is given by

$$F = -k_B T \sum_i \ln Z_i$$

where

$$Z_i = \sinh[(2s_i + 1)H_i/2k_B T]/\sinh[H_i/2k_B T].$$

The stability of the state is also checked numerically in this work.

3. Results

With the above numerical method, the H–T phase diagrams of the system can be obtained, and the results for different values of $Y = l_{Fe}/l_{Gd}$ are shown in figure 1. In these diagrams several different phases emerge and the typical spin configurations for these phases are as follows.

(i) All the Gd spins are aligned with H_0, and all the Fe spins are antiparallel to H_0: we call this state the aligned Gd state.

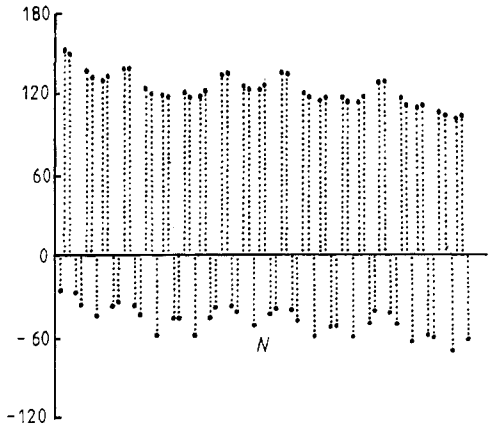

Figure 2. Variation of the twist angle θ with position. We show an entire sample of superlattice with $q = 9$, $l_{Gd} = 1$ and $Y = 2$ in a low field ($h = 0.1$) at zero temperature.

(ii) All the Fe spins are aligned with H_0, and all the Gd spins are antiparallel to H_0, we call this state the aligned Fe state;

(iii) A state where both the Gd and Fe spins are at an angle with respect to H_0. The magnitude of this angle varies with position, as illustrated in figure 2. This is the twisted state;

(iv) A state the same as the aligned Fe state except that some of the Gd spins are now also parallel to H_0, this is called the H state.

From figure 1, we see that the structure of the H–T phase diagrams is very sensitive to the change of the parameter Y. When the field h is at a low value there is a phase transition in figure 1(b) from the aligned Gd state to the aligned Fe state produced by the temperature t which varies in magnitude, but this does not appear in figures 1(a) and 1(c). In fact, for the low fields, there are always the aligned Gd or the aligned Fe states in figures 1(a) and 1(c). As the field h is increased in value, the twisted state emerges at low temperatures in all the three H–T diagrams, although the values of h_c, at which the phase transition to the twisted state happens, are different for these diagrams. These basic features of the phase diagrams can be easily understood from the viewpoint of the gain of the Zeeman energy, which would be minimised if all the spins pointed along the external field, and the exchange energy of the system, which would be minimised if all Gd were antiparallel to all Fe spins. For example, when the applied field is low, the exchange energy plays a central role and the ground state of the system should be the aligned state (the aligned Gd or the aligned Fe state) in order that the exchange energy is minimised (the ground state at low fields in figure 1(a) is the aligned Gd state instead of the aligned Fe state, since the Zeeman energy of the system is lower for the aligned Gd state than for the aligned Fe state). As the applied field is increased in value, the Zeeman energy and the exchange energy should be considered equivalently, and the competition between them finally leads to the phase transition in the system from the aligned state to the twisted state, where both the Gd and Fe spins now are at an angle with respect to the external field. The variation of this angle with position is shown in figure 2.

When the parameter Y is held constant, the phase diagrams for different values of layer number l_{Gd} are similar, but the critical field for phase transitions varies in value in these phase diagrams. The critical field h_c for the phase transition from the aligned Gd state to the twisted state at $T = 0$ as a function of the layer number $n'(=l_{Gd})$ for $q = 7$

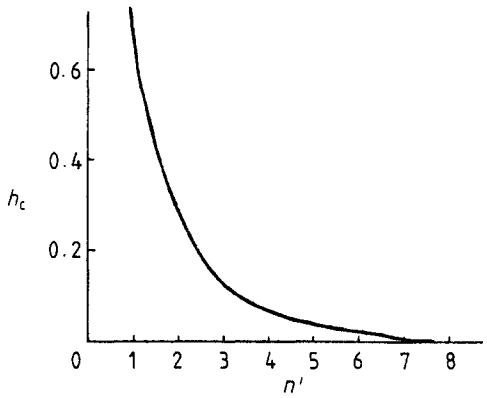

Figure 3. Critical field for the transition from the aligned Gd state to the twisted state at $t = 0$ as a function of layer number $n' = l_{Gd}$ for $Y = 1$ and $q = 7$.

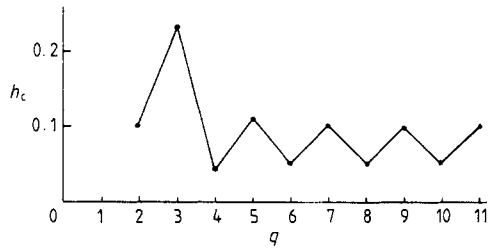

Figure 4. The critical field for the transition from the aligned Gd state to the twisted state at $t = 0$ plotted against the length of the finite quasi-periodic magnetic superlattice for $Y = 2$ and $l_{Gd} = 1$.

and $Y = 1$ is shown in figure 3. We see that the value of h_c (at $t = 0$) decreases rapidly when n' increases.

The above-mentioned phase diagrams are obtained with the length of the quasi-periodic superlattice fixed. In order to see the effect of changes of the length on the calculation results, we calculate the critical field h_c of the system with different lengths, and the results are shown in figure 4. Notice the fact that the films at both surfaces of the quasi-periodic superlattice are Gd films when q is odd and a Gd and a Fe film when q is even, and also the fact that the Gd spins are all aligned with the applied field and the Fe spins are all antiparallel to the applied field in the aligned Gd state. It is not difficult to understand that the transition from the aligned state to the twisted state produced by the increase of the applied field is easier for even q than for odd q, as indicated in figure 4. If we do not count this surface effect, changes of the length of the finite superlattice have almost no effect on the calculation results, provided the length is not too short. This can be easily seen from figure 4 where the results for all q with odd values larger than 3 are almost the same and the results for all q with even values larger than 2 are also almost the same.

In summary, we have investigated the phase transitions in finite quasi-periodic superlattices formed from magnetic films. Different kinds of equilibrium structures are obtained. It has been shown that small changes in the quasiperiodic structure can lead to dramatic changes in the H–T phase diagrams. Except for the surface effect, changes of the length of the finite superlattice have almost no effect on the calculation results when the length is not too short.

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