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Commensurate configurations in the ground state of a φ^4 model with next-nearest-neighbour interactions

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Abstract. The ground state of an extended φ^4 Hamiltonian model including next-nearest-neighbour interactions in one direction is analysed on the basis of low coupling series expansions and numerical results. It is proven that the ground state shows commensurate configurations whose wavenumbers depend on the values of the coupling constants. The model presents a ground state diagram very similar to the phase diagram obtained in the standard 3D Ising ANNNI model for $T > 0$.

One of the most commonly used models which exhibits modulated structures at $T = 0$ is the φ^4 model with anisotropic next-nearest-neighbour interactions (φ^4 ANNNI), originally introduced by Janssen and Tjon [1]. This and other related models [2–9] have been used to account for the existence of modulated phases in materials such as Na_2CO_3, $ThBr_4$, $NaNO_2$, biphenyl, etc. Previous numerical and analytical studies [1, 10, 11] of the φ^4 ANNNI model have partially elucidated the nature of its ground state configurations. In this work we give further insight into the nature and structure of the ground state by analysing the presence and stability of different configurations by means of a low coupling series expansion combined with numerical results. It is found that the ground state diagram is quite similar to the phase diagram obtained in the standard three-dimensional Ising ANNNI model at $T > 0$ [12].

The model is defined by considering scalar fields $\{\phi(\boldsymbol{r})\}$, located on the $N = L^3$ sites $\boldsymbol{r}$ of a regular lattice in three dimensions with periodic boundary conditions. The spacing a_0 of the lattice is considered to be unity. The system Hamiltonian is given by

$$\mathcal{H}(\{\phi(\boldsymbol{r})\}) = -\frac{1}{N}\sum_{\boldsymbol{r}}\{-V(\phi(\boldsymbol{r})) + J_0\ \phi(\boldsymbol{r})\left[\phi(\boldsymbol{r}+\hat{\boldsymbol{u}}_x) + \phi(\boldsymbol{r}+\hat{\boldsymbol{u}}_y)\right] + J_1\ \phi(\boldsymbol{r})\phi(\boldsymbol{r}+\hat{\boldsymbol{u}}_z) + J_2\ \phi(\boldsymbol{r})\phi(\boldsymbol{r}+2\hat{\boldsymbol{u}}_z)\} \qquad (1)$$

where $\hat{\boldsymbol{u}}_x$, $\hat{\boldsymbol{u}}_y$ and $\hat{\boldsymbol{u}}_z$ are, respectively, the unit vectors in the x, y and z directions. J_0 (assumed > 0) is the ferromagnetic coupling constant between fields located at nearest neighbour sites in the same xy plane. J_1 and J_2 are, respectively, the coupling constants between nearest and next-nearest neighbours in the z direction. The local potential $V(\phi)$ is taken to be

$$V(\phi) = -\frac{a}{2}\phi^2 + \frac{b}{4}\phi^4. \qquad (2)$$

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It is interesting to note that the usual Ising ANNNI model [12] can be obtained as a suitable limit of the model defined by the Hamiltonian (1). To this end, let us introduce new rescaled values, $S(\boldsymbol{r})$, of the fields as:

$$S(\boldsymbol{r}) = \sqrt{\frac{b}{a}}\phi(\boldsymbol{r}). \tag{3}$$

In terms of these new variables, the Hamiltonian reads:

$$\begin{aligned}\mathcal{H}(\{S(\boldsymbol{r})\}) = &-\frac{\alpha}{N}\sum_{\boldsymbol{r}}\{\tfrac{1}{2}S(\boldsymbol{r})^2 - \tfrac{1}{4}S(\boldsymbol{r})^4\} \\ &-\frac{1}{N}\sum_{\boldsymbol{r}}\{J_0'\ S(\boldsymbol{r})[S(\boldsymbol{r}+\boldsymbol{u}_x) + S(\boldsymbol{r}+\boldsymbol{u}_y)] + J_1'\ S(\boldsymbol{r})S(\boldsymbol{r}+\boldsymbol{u}_z) \\ &+ J_2'\ S(\boldsymbol{r})S(\boldsymbol{r}+2\boldsymbol{u}_z)\}\end{aligned} \tag{4}$$

where $\alpha = a^2/b$, $J_0' = J_0/a$, $J_1' = J_1/a$, $J_2' = J_2/a$. In the limit $\alpha \to \infty$, the first sum in this expression restricts $S(\boldsymbol{r})$ to take the values ± 1, and the Hamiltonian can be written as:

$$\begin{aligned}\mathcal{H}(\{S(\boldsymbol{r})\}) = -\frac{1}{N}\sum_{S(\boldsymbol{r})=\pm 1}&\{J_0'\ S(\boldsymbol{r})[S(\boldsymbol{r}+\boldsymbol{u}_x) + S(\boldsymbol{r}+\boldsymbol{u}_y)] \\ &+ J_1'\ S(\boldsymbol{r})S(\boldsymbol{r}+\boldsymbol{u}_z) + J_2'\ S(\boldsymbol{r})S(\boldsymbol{r}+2\boldsymbol{u}_z)\}\end{aligned} \tag{5}$$

which is the Hamiltonian of the Ising ANNNI model.

In studying the ground state of the Hamiltonian in equation (1), with $V(\phi(\boldsymbol{r}))$ given by equation (2), we might assume that, due to the ferromagnetic coupling between the fields located in the same xy plane, all the fields in a particular xy plane take the same value, say $\phi(z)$. This simplifies the Hamiltonian to a one-dimensional (1D) type one, namely,

$$\mathcal{H}(\{\phi(z)\}) = -\frac{1}{L}\sum_{z}\{\tfrac{1}{2}a'\phi(z)^2 - \tfrac{1}{4}b\phi(z)^4 + J_1\ \phi(z)\phi(z+1) + J_2\ \phi(z)\phi(z+2)\} \tag{6}$$

where $a' = a + 4J_0$ and b are considered to take only positive values. The constants a' and b can be included in the field scale by defining a new field $\varphi(z) = \sqrt{b/a'}\phi(z)$ such that the energy becomes (apart from a constant multiplicative factor):

$$\mathcal{H}(\{\varphi(z)\} = -\frac{1}{L}\sum_{z}\{\tfrac{1}{2}\varphi(z)^2 - \tfrac{1}{4}\varphi(z)^4 + J_1\ \varphi(z)\varphi(z+1) + J_2\ \varphi(z)\varphi(z+2)\} \tag{7}$$

where the J_1 and J_2 constants have been rescaled by a factor a'. Expression (7) is the basis of our subsequent analysis. This Hamiltonian is similar to the one obtained by Janssen and Tjon [1].

The ground state of the above Hamiltonian is found by solving the equations of the variational problem

$$\frac{\partial\mathcal{H}}{\partial\varphi(z)} = 0 \qquad \forall z = 1, \ldots, L. \tag{8}$$

This leads to a set of L coupled equations:

$$\varphi(z) - \varphi(z)^3 + J_1\ (\varphi(z-1) + \varphi(z+1)) + J_2\ (\varphi(z-2) + \varphi(z+2)) = 0 \qquad (9)$$

for $z = 1, \ldots, L$. For a given value of J_1, J_2 and L one can find, in general, many solutions of the above equations. Amongst these solutions, one has to select the one with the least energy. All the other solutions represent, in general, metastable (i.e. local minima) configurations or maxima of the Hamiltonian.

One can classify the possible system configurations, $\varphi_\lambda(z)$, according to the wavelength λ of their basic periodicity. Configurations with $\lambda = M/M'$ (M and M' natural numbers) are called commensurate. If λ is an irrational number, the configuration is called incommensurate. The search for possible solutions of equations (9) can be done in a systematic way by restricting ourselves to periodic solutions with a fixed wavelength λ, and varying λ. Let us comment that, strictly speaking, only commensurate configurations can be explicitly analysed numerically. For a given value of $\lambda = M/M'$ one has to solve the M coupled equations (9) for $z = 1, 2, \ldots, M$ (together with the periodicity conditions $\varphi(z + M) = \varphi(z)$). These solutions are composed of $2M'$ blocks. A block of length l is defined as a set of l neighbour sites with the same sign for the field φ surrounded by blocks of opposite sign (also, one of the ends of the block might take the value zero). For example, one of the solutions associated with $\lambda = \frac{14}{3}$, corresponds to the configuration $\cdots \uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\downarrow \cdots$, where $\uparrow$ ($\downarrow$) indicates a positive (negative) value for the field φ. This configuration is usually denoted by $\langle 223 \rangle$ or $\langle 2^2 3 \rangle$.

A complete search for the solutions of equations (9) can be simplified by splitting the parameter plane (J_1, J_2) into the two half-planes: $(J_1 > 0, J_2)$ and $(J_1 < 0, J_2)$. Let us remark that the Hamiltonian given by equation (7) remains invariant if one changes the sign of $\varphi(z)$ for alternate values of z and changes $J_1 \to -J_1$. This means that for a configuration with wavelength λ and any values of the pair (J_1, J_2) with energy $\mathcal{H}(J_1, J_2, \lambda)$ there exists, for the pair $(-J_1, J_2)$, a configuration with wavelength λ' such that

$$\mathcal{H}(J_1, J_2, \lambda) = \mathcal{H}(-J_1, J_2, \lambda').$$

It is easy to prove that the relationship between λ and λ' is

$$\frac{1}{\lambda} + \frac{1}{\lambda'} = \frac{1}{2} \qquad (10)$$

which is the same as that obtained in the Ising ANNNI model [13] . From now on, and due to the symmetry proved above, we restrict ourselves to the study of the half-plane $(J_1 > 0, J_2)$. If J_1 and J_2 are both greater than 0 the ground state configuration is ferromagnetic (FM), i.e. can be represented by $\lambda = \infty$. If $J_1 > 0$ and $J_2 < 0$ there is competition between both interactions and the situation is much more complicated. It is very difficult to find analytical solutions of equations (9), except for some particular cases, such as $\lambda = 4,\ 6,\ 8$ and ∞. We now consider the solutions when $J_1 > 0$ and $J_2 < 0$.

As a first step, and by analogy with the solutions found in the Ising ANNNI model, we begin by looking for constant absolute value solutions, i.e. $|\varphi(z)| = \varphi_0,\ \forall z$. In the Ising ANNNI case the parameter plane (J_1, J_2) is divided in three regions delimited by the three half lines, L1: $(J_1 = 0,\ J_2 > 0)$, L2: $(J_2 = -\frac{1}{2}J_1,\ J_1 > 0)$, L3: ($J_2 = \frac{1}{2}J_1$, $J_1 < 0$). In the region between lines L1 and L2 the ground state configuration is FM. In the region between lines L1 and L3 the ground state configuration is antiferromagnetic (AFM), and in the region between lines L2 and L3 the ground state is of 2 'up' and 2 'down' spins ($\langle 22\rangle$ configuration). This is true except for the lines L2 and L3 which are infinitely degenerate [14].

One can prove that in the φ^4 ANNNI model (and except for a few particular values of the coupling constants J_1, J_2) the only existing configurations with $|\varphi(z)| = \varphi_0$, constant, satisfying the ground state equations (9), are those having blocks of length $l_i = 1$, 2 and ∞ (which correspond, respectively, to the AFM, $\langle 22\rangle$ and FM configurations). The energy of these configurations can be exactly computed with the conclusion that the minimum energy configurations are the same as in the Ising ANNNI model, and for the same range of values of the coupling constants. The main difference is that, instead of taking the constant value 1, φ_0 depends on J_1 and J_2 as:

$$\varphi_0 = \begin{cases} \sqrt{1+2\,(J_1+J_2)} & \text{for the FM configuration} \\ \sqrt{1-2\,(J_1-J_2)} & \text{for the AFM configuration} \\ \sqrt{1-2\,J_2} & \text{for the } \langle 22\rangle \text{ configuration.} \end{cases} \tag{11}$$

Apart from the solutions described above, there are many other solutions to equations (9) that appear when we do not restrict the field values $\varphi(z)$ to take a constant absolute value. A first approach to find the ground state configuration (the solution of equations (9) with the least energy) is given by solving numerically equations (9) for different values of the parameters J_1, J_2 and comparing the energies for the solutions of different values of $\lambda = M/M'$. In practice, we have restricted ourselves to values of M that are not too large (typically $M \leqslant 30$). Of course, we cannot be absolutely sure that we have included in our numerical analysis all the relevant values for λ, and it could well be the case that another phase with a very high value for M can actually have less energy that the ones considered by us. However, that seems to us a very unlikely possibility, as supported by the structure induced by the combination mechanism discussed below. The ground state numerical solutions that we find share the two following features: (i) they are composed of blocks of length $l_i = [\lambda/2]$ or blocks of length l_i combined with blocks of length $l_j = [\lambda/2]+1$, with $[x]$ the integer part of x, (ii) the absolute minima of (7) are symmetric or antisymmetric configurations. It is possible to find many other solutions of (9), not sharing the features mentioned above, but they appear to be only local minima. Two typical configurations are shown in figure 1(a) and (b) for $\lambda = 5$ and $\lambda = 6$, respectively. Also a local minimum configuration of (7), which is neither symmetric nor antisymmetric, is shown in figure 1(c).

It was proved in a slightly different model [10] that incommensurate configurations of the form $\varphi(z) = \varphi_0 \cos(qz)$ (with the wavenumber $q \neq 0, \pi, \ldots$) are more stable than the $\langle 22\rangle$ configuration, and it was suggested that this model exhibits incommensurate states at $T = 0$. We found that this type of incommensurate structure can only exist if $|J_1/J_2| < 4$, as it takes place in the Janssen and Tjon model [10, 11]. We point out that this functional expression for $\varphi(z)$ indeed yields a more stable configuration than the $\langle 22\rangle$ for some values of the parameters J_1, J_2. However, it cannot represent the ground states of the model since it does not satisfy equations (9). Furthermore, other commensurate configurations, like the $\langle 23\rangle$ or $\langle 33\rangle$, are found to be more stable than these incommensurate states, for the different values of J_1 and J_2 that we have checked.

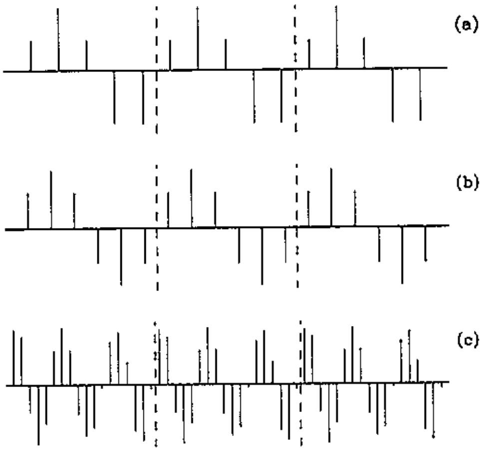

Figure 1. Typical configurations for the ground state corresponding to (*a*) $\lambda = 5$ (configuration $\langle 23 \rangle$) and (*b*) $\lambda = 6$ (configuration $\langle 33 \rangle$). In (*c*) we show the configuration $\langle 23^2 43^2 \rangle$, which, despite of being a solution of equations (9), is not a ground state configuration.

In figure 2 we show the schematic ground state diagram. This figure gives us strong evidence for the appearance of different branching processes. This is very similar to the branching processes appearing in the phase diagram of the Ising ANNNI model at $T > 0$ [15–17]. In our case, as in [16], two configurations combine to give another one. For example, the configuration $\langle 34 \rangle$ originates from the FM and $\langle 33 \rangle$ at $J_1 = 1.5957\ldots$ and $J_2 = -0.6542\ldots$.

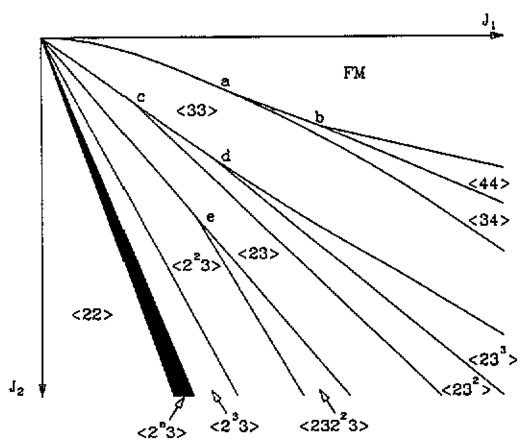

Figure 2. Schematic representation of the ground state phase diagram. Some branching points are located at the following values of (J_1, J_2): a = (1.59571,−0.65422), b = (1.81628,−0.74095), c = (0.146312,−0.08379), d = (0.45886,−0.28386), e = (0.23263,−0.14484).

It is interesting to further analyse the branching process occurring at the origin $J_1 = J_2 = 0$. In particular, it is relevant to know which configurations reach the origin and which do not. To this end, we have performed a Rth-order low coupling series expansions of configurations $\langle 2^n3\rangle$ (with $n = 1, 2, 3$), $\langle 33\rangle$, $\langle 22\rangle$, $\langle 34\rangle$, $\langle 23^2\rangle$, $\langle 44\rangle$ and the FM, as follows:

$$\varphi_\lambda(z) = \sum_{s,t=0} a_{s,t}(z,\lambda)\ J_1^s\ J_2^t \tag{12}$$

with $s + t \leqslant R$. After substitution of this expansion in equations (9) we find the coefficients $a_{s,t}(z,\lambda)$ to the desired order in J_1 and J_2 (in our case $R = 5$). Once the field values $\varphi_\lambda(z)$ have been obtained at that order, they are replaced in equation (7) to obtain the energy $\mathcal{H}(J_1, J_2, \lambda)$. By equating the energy of two different configurations we find the $J_2 = J_2(J_1)$ line which separates both configurations. For instance, the line separating configurations FM and $\langle 22\rangle$ is exactly given by $J_2 = -J_1/2$; the separating line between the FM and $\langle 33\rangle$ is: $J_2 = -J_1/2 + \frac{3}{8}J_1^2 + \mathcal{O}(J_1^3)$ and the separating line between the $\langle 33\rangle$ and $\langle 22\rangle$ is: $J_2 = -J_1/2 - \frac{3}{4}J_1^2 + \mathcal{O}(J_1^3)$ These last two separating lines differ in terms which are of order J_1^2. By studying the regions delimited by these lines we can identify which configurations exist as ground states in the neighbourhood of the origin. In general, to make sure that the configuration $\langle 2^n3\rangle$ reaches the origin we need to perform a $R = (n+2)$-order expansion. It is then proven that the configurations $\langle 2^n3\rangle$, with $n \leqslant 3$, exist as ground states for a region close to the point $J_1 = J_2 = 0$. It is then reasonable to conjecture that the configurations $\langle 2^n3\rangle$, for all n, should spring from the origin. A similar analysis also shows that the configurations FM, $\langle 22\rangle$ and $\langle 33\rangle$ spring from the same point.

One can also prove, using the series expansion, that configurations $\langle 23^2\rangle$, $\langle 34\rangle$ and $\langle 44\rangle$ are never the most stable configurations in the neighbourhood of the origin, despite being ground state configurations at the point $J_1 = J_2 = 0$ (an infinite degenerate point where all the configurations have the same energy per site $\mathcal{H} = -\frac{1}{4}$). This seems to show that configurations of the type $\langle 23^n\rangle, \langle (23)^n2^m3^p\rangle, \langle 3^n4\rangle$, etc, do not spring from the point $J_1 = J_2 = 0$. However, these configurations can appear for greater values of J_1 and $|J_2|$, as shown in figure 2.

From figure 2 it can be seen that the configurations which appear in the (J_1, J_2) ground state diagram are the same as those appearing in the phase diagram kT/J_0 versus $x = -J_2/J_1$ obtained [12] for the Ising ANNNI model at $T > 0$, and similar branching processes are observed. In particular, the branching process springing from the point $J_1 = J_2 = 0$ in the φ^4 ANNNI model is exactly the same as the branching process springing from the point ($T = 0$, $x = \frac{1}{2}$) in the Ising ANNNI phase diagram (compare figures 2 and 7 of [17] with our figure 2). Note that, in both models, only configurations of the type $\langle 2^n3\rangle$ and $\langle 33\rangle$ reach the origin.

In summary, we have studied an extension of the φ^4 model which includes next-nearest-neighbour interactions in one direction. This model has been widely used to describe the low temperature phases of some materials exhibiting commensurate–incommensurate transitions. We find that a large number of commensurate configurations appear in the ground state for different values of the coupling constants J_1 and J_2. We observe branching processes very similar to the ones obtained in the Ising ANNNI model for $T > 0$, despite of the fact that the dependence of the field φ is different from the dependence of the magnetization in the Ising ANNNI case. Our ground state diagram extends previous ground state diagrams since it includes new stable commensurate structures, some of them obtained in an analytical way. Numerical values for some branching points are also given. Further extensions of the work presented here include the study of the phase diagram of the φ^4 ANNNI model at $T > 0$. In particular, a study of the dynamics of the model [18] could help to understand the selection mechanism of the different phases at low temperatures.

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