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On partially frustrated systems

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Résumé. — Nous considérons les effets d'une frustration partielle, c'est-à-dire lorsque la frustration n'existe que dans un nombre restreint de directions de l'espace. Ces effets sont étudiés dans un modèle typique considérant un empilement de modèles d'Ising antiferromagnétiques triangulaires. A ce propos, nous étudions un modèle quantique équivalent : un modèle d'Ising bidimensionnel en champ transverse, par la méthode des tailles finies. Ils présentent tous deux de l'ordre à longue distance.

Ces considérations sont étendues aux cas où l'interaction n'est pas de type Ising avec l'idée d'application éventuelle aux phases discotiques des cristaux liquides.

Abstract. — We consider the effects of partial frustration, i.e. frustration in a restricted number of dimensions ; they are investigated in a typical model, the stacked triangular antiferromagnetic Ising model. For this purpose we studied its quantum equivalent, the 2D-triangular model with a transverse field, through finite size analysis. They both exhibit true long range order.

These considerations are extended to the non-Ising case with in mind possible application to the discotic phases of liquid crystals.

1. Introduction.

Frustration has been introduced in the context of the theory of spin glasses. These are disordered media but indeed frustration may be present in periodic systems. Various models of the latter type have been studied in recent literature and the conclusions that may be drawn are now summarized :

i) for continuous degrees of freedom (XY spins, Heisenberg spins...) the system is usually able to escape frustration and shows long range order (LRO) [1] ;

ii) in the case of discrete degrees of freedom, such as Ising models, the ground state is often highly degenerate without LRO although degeneracy is not directly linked with the absence of LRO [2, 3].

One point to be clarified is the physical relevance regarding real systems of such frustrated models (type ii) that are disordered at \( T = 0 \). Actually, on one hand, the case of discrete variables is purely ideal ; on the other hand, in periodic lattices, frustration is due to a peculiar topology of the network or to a precise distribution of interactions and is usually removed by further interactions or, more surprisingly by temperature [4].

However such configurations are not unrealistic. One example, which motivated the present work, is provided by columnar discotic phases : disk-like molecules are piled up in columns which are arranged according to a triangular lattice ; there are good reasons for assuming interactions of a frustrating type between columns. Furthermore, it is plausible, as shown in this paper, that equilibrium states are of Ising-frustrated type despite the continuous character of the order parameter.

This raises the problem of what we call « partial frustration », i.e. frustration only in a restricted number of dimensions : what is the effect of adding dimensions bearing innocent couplings ?

This article is organized as follows : in section 2 we introduce a partially frustrated model of Ising spins chosen for its simplicity ; it is equivalent to a quantum problem with a transverse field. In sec-
tions 3 and 4 the latter model is studied through finite size analysis and the results discussed in section 5. The rôle of next nearest neighbours interactions is discussed in section 6. In section 7 the problem of the density fluctuations in discotic phases is formulated; it is shown that it might lead to a highly frustrated system at low temperature.

2. A partially frustrated Ising model.

The Triangular Ising Antiferromagnet (TIA) is typical of two-dimensional frustrated models [2]. It remains paramagnetic down to \( T = 0 \). However, at \( T = 0 \), the spin-spin correlation function, averaged over all the ground states decays like a power law [7]. More precisely, considering the direction of an edge of a plaquette, the correlations decay like:

\[
\Gamma(R) \sim R^{-1/2} \cos \frac{2\pi}{3} \frac{R}{\ell}
\]

where \( R \) is the distance between spins in units of the lattice spacing. The correlation length, which is finite for \( T \neq 0 \), tends to infinity when \( T \to 0 \) : a situation which can be interpreted as a « quasi-order ».

The present model of a partially frustrated 3D system is precisely built by stacking an infinite number of TIA with a positive coupling \( J_\perp \) between neighbouring planes: see figure 1. The \( T = 0 \) situation of this model is rather peculiar: it is ordered in the direction transverse to the planes and quasi-ordered in the parallel directions:

\[
\Gamma_\parallel(R) \sim R^{-1/2} \cos \frac{2\pi}{3} \frac{R}{\ell}, \quad \Gamma_\perp(R) = 1.
\]

This motivates the investigation of the effect of temperature on such a model.

The problem may be formulated in terms of a transfer operator which acts on the states of a single TIA layer. Its exact form is rather complicated and for our purpose we limit ourselves to a simplified version relying on the concept of « weak equivalence » [8]. It states that in a particular continuum limit \( \tau \sim \beta J_\parallel \sim \exp(-2\beta J_\perp) \to 0 \) the properties of the transfer operator are those of the quantum Ising model with a transverse field:

\[
H = \sum_{ij} S_i^z S_j^z - h \sum_i S_i^x
\]

where

\[
h = (\beta J_\parallel)^{-1} \exp(-2\beta J_\perp)
\]

and where \( S^x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \) and \( S^z = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \) are spin 1/2 Pauli matrices.

The thermal behaviour of the classical 3D model is thus reduced to the non zero \( h \) behaviour of the 2D quantum model (2) at \( T = 0 \). When \( h \) is sufficiently large the ground state of (2) becomes a singlet which corresponds to the high temperature paramagnetic phase of the classical system. It is interesting to know how the system evolves from the \( h = 0 \) highly degenerate Wannier situation to the large \( h \) paramagnetic singlet ground state phase. This model has been previously studied by a real space renormalization group blocking method [9]. It was shown that the model undergoes a second order phase transition in the ground state when \( h \) passes a critical value \( h_c \).

In the following sections we would like to complete this previous study by applying another method: finite cell scaling [10]. In certain circumstances it has been shown that the finite cell scaling method could give better results than the real-space renormalization group blocking method [11]. In the present case, the method enables us to specify the nature of the ordered phase below \( h_c \) and also reveals the apparition of LRO for \( h \) infinitesimally small (\( h = 0^+ \)).

3. Finite size analysis : method.

The finite size scaling consists in solving exactly the Hamiltonian for a given sequence of finite cells of regularly increasing size and, then, in extrapolating these exact results to the infinite two dimensional lattice with help of some scaling arguments. The choice of the sequence is not obvious here since the peculiar properties of the \( h = 0 \) situation must be properly recovered when continuously increasing the size. In fact the properties of the Wannier phase are strongly sensitive to the boundary conditions. We have chosen here a sequence of triangles, with \( l \) sites on each edge. There are \( N_s = l(l + 1)/2 \) bonds (see Table I). When solving exactly the classical TIA (\( h = 0 \)) on this sequence, we find that the degeneracy \( \Omega \) of the ground state regularly increases with \( l \), as shown in table I and in figure 2 where the corresponding entropy per site \( S = \ln \Omega/N_s \) has been plotted against \( l^{-1} \). The entropy converges nicely towards the exact value \( S = 0.32306 \) of the infinite lattice [12], showing that all the Wannier states are correctly included in the ground states when going to the thermodynamic limit. We have observed that this could not be the case with other choices. For example, a sequence of squares with diagonal bonds...
Table I. — Sequence of finite cells used in the calculation. For each cell, the number of sites $N_s$, the number of bonds $N_b$, the degeneracy of the ground state for $h = 0$, $\Omega$, and the entropy per site in unit $k_B$, $S$, are reported.

<table>
<thead>
<tr>
<th>$p_z$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell</td>
<td>•</td>
<td>△</td>
<td>△</td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N_s$</th>
<th>1</th>
<th>3</th>
<th>6</th>
<th>10</th>
<th>15</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_b$</td>
<td>0</td>
<td>3</td>
<td>9</td>
<td>18</td>
<td>30</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>2</td>
<td>6</td>
<td>26</td>
<td>160</td>
<td>1386</td>
</tr>
<tr>
<td>$S$</td>
<td>0.6931</td>
<td>0.5973</td>
<td>0.5430</td>
<td>0.5075</td>
<td>0.4823</td>
</tr>
</tbody>
</table>

Moreover we have calculated the ground state spin-spin correlations function

$$\rho_{ij} = \langle S_i^z S_j^z \rangle$$

for every set of $i$ and $j$ values within the cell. The Fourier transform of $\rho_{ij}$ is analysed in the second part of the following section (§ 4.2).

4. Finite size analysis : results.

4.1 Gap. — The results of the gap are summarized in figure 3 where we have plotted $G(h)/h$ against $l^{-1}$ for different values of $h$ including the limit $h \to 0$ obtained through first order perturbation calculations. There exist some « topological » oscillations due to size effects which make the scaling analysis difficult. One observes a gap smaller than expected each time one site is located exactly at the centre of the triangle: this occurs for $l = 1, 4, 7, \ldots$. An analysis of each state shows that the topological oscillations are not present in the ground state whose energy varies regularly with $l$. They are entirely due to the first excited states which is asymmetric and which fits better when there is a node at the centre of the triangle. These oscillations become weaker when $h$ increases.

It is well known that, when a regular second order phase transition takes place in a $d$-dimensional quantum system equivalent to a $(d + 1)$-dimensional classical system, the gap plays the rôle of the inverse of the correlation length in the extra-dimension [8, 14]. In the typical example of the one dimensional Ising model in a transverse field, finite lattice calculations [15] show that the gap tends exponentially to zero or to a constant for a transverse field respectively below and above a critical value, whereas it tends to zero asymptotically in $l^{-1}$ just at the critical field. A similar behaviour is also observed in the present case from figure 3.

Fig. 2. — Plot of the entropy per site $S$ as a function of $l^{-1}$.

Fig. 3. — Numerical results for the gap: plot of $G(h)/h$ as a function of $l^{-1}$.

\[ G(h) = E_1 - E_0. \]
Apart from topological oscillations, it appears that, when $l \to \infty$, the gap tends to zero faster than $l^{-1}$ for small values of $h$ while it tends to a constant value for larger values. It is however difficult, simply looking at figure 3, to estimate the value of $h_c$ which can lie between 1 and 2. A more quantitative estimation of the critical fields is provided by the phenomenological renormalization group method [10] (PRG). An implicit renormalization group transformation which transforms $h$ into $h'$ after a size rescaling from $l$ to $l'$ is defined by:

$$lG(h) = l'G_l(h').$$

The fixed point of the transformation, which depends on $l$ and $l'$, $h_c(l, l')$ is obtained by solving the implicit equation:

$$lG(h_c) = l'G_l(h_c).$$

Better results are obtained when comparing successive sizes i.e. when taking $l' = l + 1$. Then plotting $h_c(l, l + 1)$ against the inverse of the mean size $(l + 1/2)^{-1}$ generally gives a nice convergence towards the critical field of the infinite system. This procedure has been used here and the values of $h_c(l, l + 1)$ are given by the data in figure 4. Unfortunately, here, the topological oscillations are responsible for a non-monotonic behaviour. Actually the value of $G_l$ obtained in the peculiar situation $l = 4$ cannot be compared reasonably with the neighbouring value for $l = 3$ and $l = 5$. As a consequence, we cannot have confidence in the last two points (3, 4) and (4, 5) to extrapolate $h_c(l, l')$ in the limit $l \to \infty$. These two points could conveniently be replaced by the point obtained when comparing directly $l = 3$ and $l = 5$, given by the cross in figure 4. Only a few points are left to extrapolate the results. However one can reasonably estimate $h_c$ to be in the range 1 to 3. The large error bar is here a direct consequence of the topological oscillations. The characteristic exponent $v$, which tells how the correlation length $\xi$ diverges at the transition ($\xi \sim |h - h_c|^{-v}$) can be calculated by linearizing the PRG equation (3) near its fixed point $h_c(l, l')$. This gives

$$v(l, l') = \log (l'/l)/\log \left\{ l'G_l(h_c)/G_l(h_c) \right\}$$

where $G'(h_c)$ is the derivative of the gap with respect to $h$ at $h = h_c(l, l')$. Applying the same extrapolation procedure as that used for $h_c(l, l')$ to the L.H.S. of figure 4, leads to a value of $v$ in the range 0.5 to 1.5.

This exponent tells also how the gap closes at $h_c$ in the infinite system since $G \sim |h - h_c|^s$ with $s = vz$. Here $z = 1$, thus $s = v$.

The previous values obtained through a renormalization group method [9] $h_c \sim 1.4$, $v \sim 0.8$ are not so different. As usual, when comparing both methods it is better to trust the finite-cell scaling results which take into account larger cells [10, 11].

Even if the numerical estimations of $h_c$ and $v$ are imprecise due to the topological oscillations, one can certainly exclude any pathological behaviour such as $h_c = 0$ or $v^{-1} \to 0$. Thus, from the PRG analysis one can conclude that a « regular » second order phase transition with finite exponents takes place at a non-zero $h_c$ value. There is certainly no peculiar marginal behaviour at $h_c$ such as an essential singularity like in the classical 2D XY model [16]. Notice that the estimated $v$ exponent for the regular ferromagnetic Ising model in three dimensions (equivalent to the ferromagnetic Ising model in a transverse field in two dimensions) is $v \sim 0.63$ [17], located inside the error bars of our estimation.

### 4.2 CORRELATION FUNCTIONS.

In order to specify the nature of the low field phase and, in particular, to decide whether there is some long range magnetic...
order or not, we have calculated for each finite cell the pseudo-Fourier transform of the spin correlation function in the ground states defined here as a simple double sum over the sites:

$$\rho(q) = \frac{1}{N^2} \sum_{ij} \rho_{ij} \exp(iq \cdot \mathbf{R}_{ij}) = \frac{1}{N^2} \sum_{ij} \langle S_i^z S_j^z \rangle \exp(iq \cdot \mathbf{R}_{ij})$$

where $\mathbf{R}_{ij} = \mathbf{R}_j - \mathbf{R}_i$ is the vector in the direct space connecting sites $i$ and $j$. We have investigated the full Brillouin zone of the triangular lattice and we give here some characteristic results under the form of a plot of $\rho(q)$ along the directions OA, OB and BA defined in figure 5. In principle, if any long range magnetic order develops in the thermodynamic limit, one must observe the appearance of some peak around a given wavevector $q_0$.

Let us first present the calculations in the peculiar case $h = 0$ where the system is entirely classical (i.e. $S_i = \pm 1$). In that case, each of the degenerate ground states must be given the same weight and then, the correlation function corresponds to a simple average over the Wannier states $\omega = 1, 2, ... \Omega$

$$\rho_{ij} = \Omega^{-1} \sum_{\omega} \langle S_i^z S_j^z \rangle_{\omega}$$

The resulting spectrum is given in the top of figure 6. An absolute maximum occurs at wavevector $q_B$, a saddle point at $q_A$ and an absolute minimum is located at $q_0$. $q_B$, $q_A$ and $q_0$ correspond respectively to points B, A, 0 of the Brillouin zone (see Fig. 5). The intensities $\rho_B$, $\rho_A$, $\rho_0$ at these points are plotted against $l^{-1}$ on the right part of the figure. All these intensities tend to zero when $l \to \infty$ showing that no peak is developed in the thermodynamic limit. This is consistent with the exact result that there is no long range order at $T = 0$ in the TIA model [7, 12].

**Fig. 5.** Direct space (a) and reciprocal space (b) showing the Brillouin zone of the triangular lattice with peculiar points O, A, B.

**Fig. 6.** Results for the correlation functions. The quantity $\rho(q)$ is plotted along the lines OA, OB, BA (left) and the intensities $\rho_B$, $\rho_A$, $\rho_0$ at point O, A, B have been plotted as a function of $l^{-1}$ (right).

Top, centre and bottom of the figure correspond respectively to the results for $h = 0, 0^+$ and $h = 0.5$. 

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The results obtained through the first order perturbation calculation (i.e. with infinitesimal \( h \)) are represented. The difference with the calculation above is that the correlation function is no longer a simple average but actually an expectation value taken in the right combination of the Wannier states corresponding to the ground states for \( h = 0^+ \). The ground state is now given by:

\[
\psi_0 = \sum_{\omega} a_\omega \left| \omega \right> .
\]

The coefficients \( a_\omega \) are determined numerically in the limit of first order perturbation \((h \rightarrow 0)\) and the correlation function is calculated as:

\[
\rho_{ij} = \Omega^{-1} \sum_{\omega} |a_\omega|^2 \langle S_i^z S_j^z \rangle_{\psi_0} .
\]

Results for the spectrum are given in the center of figure 6. The same general shape with a maximum at \( q_B \) is observed. However, while \( \rho_{pp} \) and \( \rho_{00} \) tend to zero when \( l \rightarrow \infty \), the intensity of the maximum \( \rho_{bb} \) clearly tends to a non zero value in contrast with the preceding situation. One can estimate

\[
\rho_{bb}^0 \approx 0.24 \pm 0.01
\]

as being the square of the spontaneous magnetization. This result suggests the occurrence of LRO with modulation \( q_B \) in the infinite system. The direction of the modulation corresponds to a basal direction of one unit triangle of the direct lattice. The intensity of the modulation is \( |q_B| = \frac{4\pi}{3a} \), if \( a \) is the length of the side of a triangle. The corresponding wavelength is \( 3a/2 \) in the direct space. (A classical example of such ordering is given by the sequence 0, +, −, 0, +, ...)

Finally, we present the general results for \( \rho_{ij} \) for different non zero values of \( h \) by calculating the expectation value in the ground state of the full Hamiltonian \((2)\). The results are given in figure 6 (bottom) and figure 7. For small \( h \) values, one can observe qualitatively the same behaviour as for \( h = 0^+ \). However the estimated spontaneous magnetization decreases when \( h \) increases. For larger \( h \) values, one observes a different behaviour : all the intensities \( \rho_{pp}, \rho_{AA}, \rho_{BB} \) tend to zero when \( l \rightarrow \infty \). The change of behaviour occurs about \( h \approx h_c \approx 2 \). This strongly suggests that the transition at \( h = h_c \) corresponds to the long range magnetic order. Unfortunately, our precision is not sufficient to give an estimation of the exponent \( \beta \) which tells how the magnetization tends to zero at \( h = h_c \). Moreover, note that whereas the peak stays at \( q = q_B \) as long as \( h \) is lower than \( h_c \), it shifts towards lower \( q \) values in the paramagnetic phase for \( h > h_c \). The same effect was obtained by Stephenson for the correlation function of the TIA at finite temperature.

5. Discussion.

The finite cell study of the quantum 2D TIA shows that, when applying an infinitesimal transverse field, LRO sets in and remains up to a critical value \( h_c \). This LRO is defined by wavevectors such as \( q_B \) (Fig. 5). Moreover Stephenson’s result is also completed by establishing that the TIA exhibits at \( T = 0 \), \( h = 0 \), a quasi order (pseudo Bragg peak) of antiferromagnetic type and not only a slowly oscillating decay of the correlations as in \((1)\). The associated pseudo-Bragg peak turns into a true Bragg peak as soon as \( h \) is different from zero.

Thus, going back to the 3D model, from which we started, we can now assert that for \( 0 < T < T_c \) it shows a periodic LRO of wave vector \( q_B \) and that:

\[
\lim_{T \rightarrow 0} |\langle S_i^z \rangle| \neq 0
\]

at least when the weak equivalence holds, i.e. in the strong anisotropy limit.

Such a situation where temperature favors order has already been encountered in a 2D case [4]. Probably the same phenomenon occurs in the antiferromagnetic Ising f.c.c. lattice [18]. This is reminiscent of what happens in weakly coupled XY planes : an infinitesimal interplane coupling changes quasi-order.
into LRO. The results obtained in the framework of the quantum equivalence can be interpreted directly in the classical 3D model by the following low temperature analysis. Let $| \alpha \rangle$ be a state of the TIA and denote by $\alpha$ the vector of $\mathbb{R}^N$, if $N_\parallel$ is the number of sites in each layer:

$$\alpha = \{ \alpha_i \} \quad \alpha_i = \langle \alpha | \sigma_i | \alpha \rangle \quad 1 \leq i \leq N_\parallel.$$ 

Then the partition function is:

$$Z = \sum_{\alpha_1, \ldots, \alpha_N} \exp - \beta \sum_\alpha \{ E_{\text{TIA}}(\alpha_\alpha) - J_\perp \alpha_\alpha \alpha_{\alpha+1} \}.$$ 

One may eliminate every second layer by performing the summation over the states of odd indice planes: one is left with:

$$Z = \sum_{\alpha_2, \ldots, \alpha_N} \exp - \beta \sum_\alpha \{ E_{\text{TIA}}(\alpha_2\alpha) + F_{\text{TIA}}(J_\perp \alpha_2\alpha + J_\perp \alpha_2\alpha_+2) \}.$$ 

$F_{\text{TIA}}(h)$ is exactly the free energy of the TIA in the presence of a distribution of fields $h = \{ h_i \}$. This defines the hamiltonian for the renormalized system. $F_{\text{TIA}}(h)$ is not exactly known but it is very useful in view of Stephenson's results, it is legitimate to assert that for $T \to 0$, $F$ is minimum for fields $h$ of the form $h_i \propto \exp(iq^B \cdot R_i)$. Therefore states $\alpha_{2\alpha} = \alpha$ with wavevectors like $q^B$ are favoured, even at $T = 0^+$, by thermal agitation. In this way the degeneracy of the Wannier states is reduced. This assertion can be made rigorous in the limit $T = \text{const.} \neq 0, J \to 0$ where $F$ may be expanded:

$$F_{\text{TIA}}(2J_\perp \alpha) \approx F_{\text{TIA}}(0) - \sum_q \chi_q |2J_\perp \alpha_q|^2 + \cdots.$$ 

The expression (1) for the spin correlation function implies that:

$$\chi_q = \beta \sum_U \langle S_i S_j \rangle \exp iq(R_i - R_j)$$

is maximum for $q = q_B$ which achieves our proof.

While preparing this manuscript we received a preprint by Blankschtein et al. [19] who considered the same model. Their results confirm ours apart from the fact that they predict 2 phase transitions. This is not incompatible with the present analysis for 2 possible reasons:

1) The 2 ordered states differ only through a change of phase so that our $\rho(q)$ study cannot differentiate between them.

2) The weak equivalence is only valid for large $J_1$; in this limit it may be supposed that the low temperature phase shrinks and vanishes at $T = 0$. In the next section, we investigate the stability of these results with respect to the addition of next nearest neighbours interactions.

6. Role of next-nearest neighbours.

Consider the Ising model on a triangular lattice with nearest neighbours exchange $J_1 < 0$ and n.n.n. exchange $J_2$. The ground states are easily found and are depicted in figure 9 for both negative and positive $J_2$. They are sixfold degenerate ferrimagnetic for $J_2 > 0$, antiferromagnetic for $J_2 < 0$. We have performed finite size calculations of $\rho(q)$ like in section 4 but, here, only for $h = 0$ and $h = 0^+$. For positive n.n.n. couplings ($J_2 > 0$) the results, which are similar for $h = 0$ and $h = 0^+$ are reported in figure 10. When $l \to \infty$, we recover a strong Bragg peak at $q_B$ and a smaller extra Bragg peak at $q = 0$ (another peak located between 0 and $A$ disappears when $l \to \infty$). This result is consistent with the ferrimagnetic structure of figure 9b. For negative n.n.n. couplings ($J_2 < 0$) the results are slightly different for $h = 0$ (Fig. 11a) and $h = 0^+$ (Fig. 11b) but it seems that the same situation is recovered when $l \to \infty$ in both cases: only one strong Bragg peak remains at $q = q_A$, while the other two small peaks at $q = 0$ and in between $q = 0$ and $q = b_B$ disappear when $l \to \infty$ (this is not so clear in the case $h = 0^+$ : the peak located between $q = 0$ and $q = q_B$ in only slightly smaller for $l = 5$ compared with $l = 4$ and unfortunately the results for $l = 6$ are not available). A single peak at $q = q_A$ is consistent with the antiferromagnetic
structure of figure 9a. Thus the finite cell calculations for \( h = 0 \) confirm the expected structure (Fig. 9a) in presence of n.n.n. couplings. Moreover the results for \( h = 0^+ \) show that these structures persists in presence of a transverse field and consequently, at finite temperature, in the classical equivalent.

The same kind of LRO structures have been found by Fujiki et al. [20] and Takyama et al. [21]. However, the same authors claim that when temperature increases in the case \( J_2 > 0 \), the above ferromagnetic phase is followed by a quasi-order state of \( XY \) like type. In view of predominant size effects, the existence of such a phase cannot be taken for granted, neither a finite \( T_c \) when \( J_2 \rightarrow 0 \).

7. Columnar phases: a partially frustrated system.

For a review on columnar liquid crystals see (5) and references therein. A discotic phase is pictured on figure 8a. The disc like molecules are oriented parallel to the \( x-y \) plane (nematic order) but this paper will not be concerned with this degree of freedom. Let the position of the centre of mass of the \( n \)th molecule be \( \mathbf{R}_n \). The \( x-y \) projection of \( \mathbf{R}_n \) shows a LRO defined by a triangular lattice, whereas there is no LRO for the \( z \) projection. The system may be viewed as made of \( \omega \) columns inside which the molecules are free. In such phase the system has a tendency to become a true crystal with a given lattice spacing along \( z \) of \( 2 \pi/Q \).
The associated fluctuations will be described by complex fields \( \psi_i(z) \) related to the density of the centres of mass \( \rho_i(z) \)
\[
\rho_i(z) = e^{i\omega z} \psi_i(z) + e^{-i\omega z} \psi_i^*(z)
\]
where index \( i \) labels the sites of the triangular lattice (or the columns). The Ginzburg-Landau free energy functional can generally be written as
\[
\mathcal{F} = \mathcal{F}_c + \mathcal{F}_{\text{int}}
\]
where \( \mathcal{F}_c \) is the contribution of isolated columns and \( \mathcal{F}_{\text{int}} \) represents the interaction between neighbouring columns. The classical form for \( \mathcal{F}_c \) is
\[
\mathcal{F}_c = \int dz \sum_i \left( a |\psi_i(z)|^2 + b |\psi_i(z)|^4 + c \left| \frac{d\psi_i(z)}{dz} \right|^2 \right).
\]
Clearly this problem is analogous to that of superconducting filaments \([6, 23]\). It is well known that only phase fluctuations are important and we will consider that \( a < 0 \) so that \( |\psi| \sim \psi_0 \) and \( \psi_i(z) = \psi_0 e^{-i\phi_i(z)} \) thus:
\[
\mathcal{F}_c = \text{Const.} + c\psi_0^2 \sum_i \left| \frac{d\psi_i(z)}{dz} \right|^2.
\]
Let us now discuss the interaction term \( \mathcal{F}_{\text{int}} \). Probably the interaction between columns, which is of steric origin, is repulsive. For an isolated pair of columns the expected configuration is the one of figure 8b i.e. with a phase difference of \( \pi \) and the following simple form for \( \mathcal{F}_{\text{int}} \) may be proposed:
\[
\mathcal{F}_{\text{int}} = -K \sum_{\langle ij \rangle} |\psi_i(z)\psi_j^*(z)| + \text{c.c.}
\]
where \( \langle ij \rangle \) are nearest neighbours.
This is the analog of the Josephson coupling in the context of superconductivity (but here with the opposite sign).

Minimizing \( \mathcal{F} \) amounts to finding the ground states of the \( XY \) triangular antiferromagnetic model. In this case it has been shown \([1]\) that frustration does not prevent LRO: the system is a three-sublattice antiferromagnet. Such a configuration has been observed in the crystal phase of some triphenylene-esters where aliphatic chains are short \([22]\). The structures of 2 neighbouring columns differ in phase by \( 2\pi/3 \) so that this state is well described by a phase variable \( \phi_i(z) \) obeying Hamiltonian (4) with \( K < 0 \).
However the quadratic interaction (4) is justified only if lowest order terms in \( \psi \) may be retained, that is, if \( \psi_0 \) is small. When the coupling is strong, and this is probably the case in most experimental situations where the aliphatic chains are longer, the potential is more complicated than (4) and higher order harmonics in \( \phi_i - \phi_j \) must be taken into account. It is shown below that, in certain cases, the ground states may have the same structure as in the Ising model (Wannier states): frustration is much more efficient than in the usual \( XY \) model. Consider the general form for \( \mathcal{F}_{\text{int}} \)
\[
\mathcal{F}_{\text{int}} = \int dz \sum_{\langle ij \rangle} f(\phi_i - \phi_j)
\]
where \( f \) is a \( 2\pi \)-periodic function, symmetrical with respect to 0 and \( \pi \) and having an absolute minimum at \( \pi \). First look for the minima of \( H = \sum_{ij} f(\phi_i - \phi_j) \) on a triangular lattice. As usually, this is achieved by separate minimization over each triangular plaquette. The stationarity condition requires:
\[
- f'(\phi_3 - \phi_2) + f'(\phi_2 - \phi_1) = 0.
\]
Generally the solutions fall into two classes:
- Class 1 : \( \phi_3 - \phi_2 = \phi_2 - \phi_1 = \pm 2\pi/3 \). These yield the ground states of the genuine \( XY \) model \([1]\).
- Class 2 : \( \phi_i - \phi_j \) takes the values 0 or \( \pi \). It is convenient to introduce Ising spins \( \sigma_j \) in the following way:
\[
\phi_i = \alpha + \frac{\pi}{2} \sigma_i
\]
with respect to an arbitrary direction \( \alpha \). Then:

\[
\mathcal{K} = \sum_{\langle ij \rangle} f \left( \frac{\pi}{2} \sigma_i - \frac{\pi}{2} \sigma_j \right) = \sum_{\langle ij \rangle} \left( \frac{f(0) + f(\pi)}{2} + \frac{f(0) - f(\pi)}{2} \sigma_i \sigma_j \right).
\]
The ground states in this class are precisely the (degenerate) Wannier states since \( J = \frac{1}{2} (f(\pi) - f(0)) < 0 \). It is immediately seen that if the depth of the potential is such that:
\[
2 f(\pi) + f(0) < 3 f(2\pi/3)
\]
these states have a lower energy than those of class 1. This shows that with continuous variables, frustration may lead to a large number of states; the present model is quasi-ordered in the \( x-y \) plane and ordered in the \( z \) direction at \( T = 0 \).
The effect of temperature is, a priori, different from the true Ising case since the elementary excitations are of another type: they consist of small tilts $\theta_i(x)$ of the spins, as described in what follows:

$$\phi_i(x) = \alpha + \frac{\pi}{2} \sigma_i + \theta_i(x).$$

The free energy will be expanded about each minimum defined by (5)

$$\mathcal{F} = \sum_{\langle ij \rangle} f\left(\frac{\pi}{2} \sigma_i - \frac{\pi}{2} \sigma_j\right) + \frac{1}{2} \sum_{\langle ij \rangle} f''\left(\frac{\pi}{2} \sigma_i - \frac{\pi}{2} \sigma_j\right)(\theta_i - \theta_j)^2$$

$$= \text{const.} - J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \sum_{\langle ij \rangle} (A + B \sigma_i \sigma_j)(\theta_i - \theta_j)^2.$$

The partition function, at low $T$ is the sum of the contributions of each ground state and the small fluctuations associated with each of them:

$$Z \propto \sum_{\mathcal{W}_S} \prod_i \mathcal{D}\theta_i(x) \exp - \beta \int dz \left( \sum_{\langle ij \rangle} (A + B \sigma_i \sigma_j)(\theta_i - \theta_j)^2 + \sum_i c\psi_i \frac{d\theta_i}{dz}^2 \right)$$

$$\sum_{\mathcal{W}_S} \text{stands for summation over configurations of } \sigma_i \text{ which are Wannier states. Fourier transforming along the } z \text{ direction:}$$

$$Z \propto \sum_{\mathcal{W}_S} \prod_i \mathcal{D}\theta_i \exp - \beta \left( \sum_{\langle ij \rangle} (A + B \sigma_i \sigma_j) |\theta_i - \theta_j|^2 + \sum_i c\psi_i k^2 |\theta_i|^2 \right).$$

Changing $\theta \rightarrow \beta^{1/2} \theta$ in the integrations above, it is readily seen that thermal fluctuations bring on an extra interaction $\mathcal{U}(|\{ \sigma_i \}|)$ which is independent of temperature:

$$Z \propto \sum_{\mathcal{W}_S} \exp - \mathcal{U}(\{ \sigma_i \}), \quad (6)$$

and which yields a statistical distribution spread over the Wannier states instead of removing the degeneracy as in part 6 for n.n. neighbours. Whether some LRO would originate from (6) is not straightforward; on one hand because the complete expression of $\mathcal{U}$ is intricate involving long range and multispin couplings, on the other hand because the summation in (6) runs only over the Wannier states.

For these reasons we limit ourselves to a lowest order expansion in $B$ and to a mean field treatment of (6) restricted to the Wannier subspace. To second order in $B$ we have:

$$- \mathcal{U}(\{ \sigma_i \}) = \frac{B^2}{2} \sum_{\langle ij \rangle} 2 \sigma_i \sigma_j - \sum_{\langle i \rangle} A |\theta_i|^2 + \sum_{\langle j \rangle} c\psi_j k^2 |\theta_j|^2$$

(7)

$$\langle \cdots \rangle_0 = (\text{normalization}) \times \int d\theta_i \ldots \exp - \sum_{\langle k \rangle} A |\theta_i|^2 - \sum_{\langle l \rangle} c\psi_l k^2 |\theta_l|^2$$

$$A_{ij}^2 = \sum_{\langle k \rangle} (|\theta_i| - |\theta_k|^2 - \langle |\theta_i| - |\theta_k|^2 \rangle_0).$$

(The average value has been subtracted in the definition of $A_{ij}^2$ because it yields a constant in $\mathcal{U}$ when considering only Wannier states). Expression (7) contains two-spins and four-spins interactions which are made explicit below:

$$\mathcal{U}(\{ \sigma_i \}) = - K_1 \sum_i \sigma_i \sigma_{i+\mathbf{A}} - K_2 \sum_i \sigma_i \sigma_{i+2\mathbf{A}} - \sum_{ijlm} \sigma_i \sigma_j \sigma_{i+\mathbf{A}} \sigma_{j+\mathbf{A}}$$

with the definitions:

$$\langle \cdots \rangle_0 = (\text{normalization}) \times \int d\theta_i \ldots \exp - \sum_{\langle k \rangle} A |\theta_i|^2 - \sum_{\langle l \rangle} c\psi_l k^2 |\theta_l|^2$$

$$A_{ij}^2 = \sum_{\langle k \rangle} (|\theta_i| - |\theta_k|^2 - \langle |\theta_i| - |\theta_k|^2 \rangle_0).$$

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(8)

$$K_1 = \frac{B^2}{2} \sum_{\mathbf{k}} \langle \theta_{i+\mathbf{A}} \rangle^2$$

(9)

$$K_2 = \frac{B^2}{2} \sum_{\mathbf{k}} \langle \theta_{i+\mathbf{A}} \theta_{i-\mathbf{A}} \rangle^2$$

(9)
(See Fig. 12 for the definitions of the translation vectors $\mathbf{a}$ and $\mathbf{A}$). In the mean field approximation the wave vector dependent susceptibility of the fictitious spin $\sigma$ is

$$\chi^{-1}(q) = \chi_0^{-1}(q) - K(q)$$

where $\chi_0$ is the ground state susceptibility of the TIA model which is known to have the property $\chi_0^{-1}(q_{B}) = 0$.

A straightforward calculation from (8) shows that

$$K(q_{B}) = 6 K_1 - 3 K_2 .$$

We have calculated $K_1$ et $K_2$ in the continuum approximation, i.e. assuming in (9) and (9') that $\mathbf{a}$ and $\mathbf{A}$ are small and that the Brillouin zone is isotropic. In that case one finds exactly $K(q_{B}) = 0$ which would imply that the algebraic decay (1) remains. Indeed this result is probably not valid beyond this approximation. We do not feel it would be very instructive to go further and calculate $K_1$ and $K_2$ exactly because the above treatment is rather crude by itself. However it reveals that the actual situation is not very far from the marginal case of the pure TIA model : this is the fact we would like to retain from this analysis.

8. Conclusion.

We have considered different possibilities of partial frustration in 3D periodic systems. This notion seems to be physically sound and in particular is not restricted to the ideal case of Ising spins. From the experimentalist's viewpoint, total absence of LRO as a manifestation of frustration — partial as well as total — is probably difficult to observe. However a succession of several ordered phase and eventually reentrance, is rather generally a consequence of frustration.

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