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Commensurate phases for a two-dimensional non-linear lattice

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Abstract. We consider a two-dimensional (2D) hexagonal lattice model with two sites per cell and an on-site double-quadratic potential, where harmonic interactions are taken into account. We present a simple calculation procedure for obtaining the static solutions of *atomic positions* for all the commensurate phases of the model. We derive a detailed phase diagram which demonstrates the validity of these solutions, and which exhibits some new features of the model which are evident when comparisons with previous work are made.

1. Introduction

1D and 2D non-linear lattices have been intensively investigated to model some phase transitions in various materials such as LiIO_3 [1] NaNO_2 or $\text{SC}(\text{NH}_2)_2$ [2–4] domain walls in ferroelectric and antiferroelectric crystals [5, 6], spatially modulated systems, [7–11], incommensurate phases [12] or chaotic states [13–15]. The calculational procedures of static solutions for the *isolated wall structures* [1, 6, 9], the commensurate phases [7–9] and the chaotic states [13–15] have been set up for classical 1D models. However, all these calculations are difficult to extend to 2D non-linear lattice models because of their complexity. The main problem in determining the static structures of these 2D models lies in calculating the *atomic positions*, from which the energy of the structure is derived. To our knowledge, the commensurate static solutions for the 2D models treated so far have been always obtained only for simple phases with lower period or higher symmetry [1, 16–19]. This restriction to only such phases generally allows one to solve almost all the mathematical problems but provides obviously only partial results, so that very often the phase diagrams (PD) for 2D models are oversimplified. That is, that they show a great variety of quasi-1D phases and only a few ‘true 2D phases’ [1, 17, 18]. In [17], Büttner and Heym considered a triangular lattice with an on-site double-quadratic substrate potential. Their PD shows two *true* 2D phases. Vlastou-Tsinganos *et al* [18] examined a trigonal lattice with an on-site ϕ^4 substrate potential. In the PD that they obtain, one finds only one *true* 2D phase. Coquet *et al* [1] investigated a hexagonal lattice. No *true* 2D phase appears in the PD obtained by the latter (where only quasi-1D phases are present). However, it should be mentioned that lengthy calculations are usually needed to obtain the static solutions for the *true* 2D phases. It is

then fairly tedious to derive a detailed PD which necessitates that a great number of *true* 2D phases are examined.

In the present paper we present a simple calculational procedure for obtaining the static solutions for *atomic positions* for all the commensurate phases of a classical 2D non-linear lattice. We consider the hexagonal lattice examined recently by Coquet *et al* [1] to study some phase transitions in lithium iodate, described in detail in section 2. Besides the fundamental interest of this model, it should be stressed that it provides a fairly complete description of the different enantiomorphic forms of the α -phase and the α -to- γ transition of LiIO_3 , as discussed in [1]. This crystal has been intensively investigated from an experimental point of view, owing to its non-linear optical properties. It has also attracted new interest in particular for its structural phase transitions [1, 20–22]. Three modifications of LiIO_3 are known; upon heating, α - LiIO_3 (i.e. the α -phase of LiIO_3) transforms reversibly into γ - LiIO_3 (at about 500 K with a large hysteresis), and then γ - LiIO_3 transforms irreversibly into β - LiIO_3 (at 540 K) which is stable up to the melting point (768 K). Further details about LiIO_3 can be found in [1, 20–24]. The model under consideration also provides the possibility of some useful extensions such as the study of finite systems in an attempt to explain some grain size effects on the phase transition temperatures observed in LiIO_3 .

In the present paper, we show that each commensurate phase $P_n * P_m$ (i.e. with periodicity P_n and P_m respectively in the two *directions* n and m of the lattice) with configuration σ (sequence of Ising variables ± 1 describing the occupied side of the double-well substrate potential at each cell of the lattice) can be characterized by a matrix $\mathbf{M}(P_n, P_m)$ from which the *atomic positions* are derived in a straightforward manner by elementary calculations. We present the matrices $\mathbf{M}(P_n, P_m)$ for all the commensurate phases of the model. The main virtue of this calculational procedure is that it enables us to investigate any commensurate phase of the model, unlike previous work [1] where the static solutions are calculated only for the $2 * 2$ phases. Moreover we re-emphasize that no *true* 2D phase appears in the PD obtained in [1], shown in figure 1, where one finds only a few quasi-1D phases. The PD that we obtain in the present work preserves most of the main conclusions drawn in [1] and therefore demonstrates the validity of our commensurate static solutions $\mathbf{M}(P_n, P_m)$, but our calculational procedure

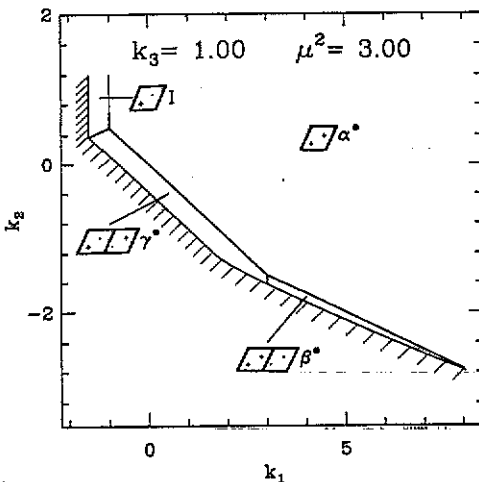


Figure 1. Plot of the PD obtained by Coquet *et al* [1].

is more general in that our PD shows a great variety of *true* 2D phases, and also some quasi-1D phases. Moreover, as discussed later, our results show that the hexagonal model under consideration cannot even partially provide, as claimed in [1], a description of β -LiIO₃, or the γ -to- β transition of LiIO₃. On the other hand our PD exhibits a special feature of the model, i.e. is a re-entrant behaviour which occurs in some parameter regions with a re-entrant *true* 2D phase. This unusual phenomenon has been already observed for nematic and smectic phases of some liquid crystalline materials with cyano derivatives [25–27] and also in a quasi-1D system, described by two coupled Ising order parameters [28].

The paper is organized as follows. In section 2 we describe the model and we calculate the matrices \mathbf{M} (P_n, P_m) for all the commensurate phases of the model. We also stress the ease with which the static solutions are derived from this calculational procedure. In section 3 we obtain the PD. In section 4 we compare our PD with the other work and discuss the new features of the model, and in section 5 we summarize our results.

2. General solutions

The model is schematically shown in figure 2, where two sites $i = 1, 2$ lie at positions $(\frac{2}{3}, \frac{1}{3})$, $(\frac{1}{3}, \frac{2}{3})$ in each cell. (The relationship between LiIO₃ and the hexagonal model under consideration is discussed in detail in [1].) The cells are labelled by indices, n, m and each site is characterized by an angle $q_{n,m,i}$ which represents the rotational position of an iodate ion of LiIO₃, as we discuss later, which we call henceforth '*atomic position*' to use a more usual terminology. There exists for each *atomic position* of IO₃⁻ ions two possible equilibrium configurations. This physical behaviour is generally modelled by assuming an on-site double well potential [1, 20, 21], chosen in [1] with a double quadratic shape:

$$P = \frac{1}{2}\mu^2(q_{n,m,i} - \epsilon\sigma_{n,m,i})^2$$

where $\epsilon^2\mu^2/2$ measures the potential barrier, $\sigma_{n,m,i} = \text{sgn}(q_{n,m,i})$, and $\pm\epsilon$ locates the two minima of the potential. A site n, m of type i ($i = 1, 2$) is connected to neighbouring sites by harmonic interactions of constant k_1 to the three nearest neighbours of the second type, k_2 with the six nearest neighbours of the same type i and k_3 with the three second neighbours of the opposite type. We assume the same symmetrized form of the energy

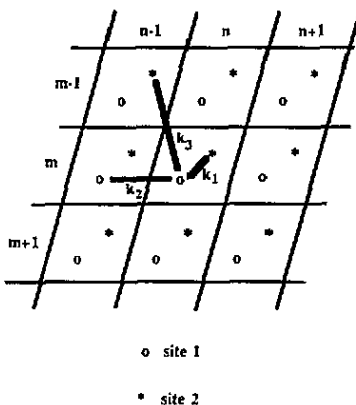


Figure 2. The hexagonal 2D lattice model under consideration.

per site as that considered in [1]. The static structure of the system is obtained by energy minimization, which gives the following equilibrium equations for each site:

$$\begin{aligned}
 & [\mu^2 + 3(k_1 + k_3) + 6k_2]q_{n,m,1} - k_1(q_{n,m,2} + q_{n,m-1,2} + q_{n+1,m,2}) \\
 & \quad - k_2(q_{n-1,m,1} + q_{n-1,m-1,1} + q_{n,m-1,1} \\
 & \quad + q_{n+1,m,1} + q_{n+1,m+1,1} + q_{n,m+1,1}) \\
 & \quad - k_3(q_{n-1,m-1,2} + q_{n+1,m-1,2} + q_{n+1,m+1,2}) = \epsilon\mu^2\sigma_{n,m,1} \quad (2.1a)
 \end{aligned}$$

$$\begin{aligned}
 & [\mu^2 + 3(k_1 + k_3) + 6k_2]q_{n,m,2} - k_1(q_{n,m,1} + q_{n,m+1,1} + q_{n-1,m,1}) \\
 & \quad - k_2(q_{n-1,m,2} + q_{n-1,m-1,2} + q_{n,m-1,2} \\
 & \quad + q_{n+1,m,2} + q_{n+1,m+1,2} + q_{n,m+1,2}) \\
 & \quad - k_3(q_{n-1,m-1,1} + q_{n+1,m+1,1} + q_{n-1,m+1,1}) = \epsilon\mu^2\sigma_{n,m,2}. \quad (2.1b)
 \end{aligned}$$

We start from equations (2.4) already obtained in [1], and we use a two-step process to derive the general solution for a commensurate phase $P_n * P_m$ with configuration σ .

(i) We rewrite the above equilibrium equations with the periodicity condition in m :

$$q_{n,m,i} = q_{n,m+P_m,i} \quad (2.2)$$

which gives us a system of $2P_m$ equations which we transform into the following matrix equation:

$$\mathbf{A}(P_m)\mathbf{U}_{n-1}(P_m) + \mathbf{B}(P_m)\mathbf{U}_n(P_m) + \mathbf{A}(P_m)^T\mathbf{U}_{n+1}(P_m) = \mathbf{D}_n(P_m) \quad \text{for all } n \quad (2.3)$$

where $\mathbf{U}_n(P_m)$ and $\mathbf{D}_n(P_m)$ are the $2P_m \times 1$ (column) matrices respectively for the *atomic positions* and the configuration σ , listed in table 1. The superscript T denotes the transpose matrix; $\mathbf{A}(P_m)$ and $\mathbf{B}(P_m)$ are $2P_m \times 2P_m$ matrices defined as follows:

$$\begin{aligned}
 \mathbf{A}(1) &= \begin{pmatrix} -2k_2 & -(k_1 + 2k_3) \\ -k_3 & -2k_2 \end{pmatrix} \\
 \mathbf{B}(1) &= \begin{pmatrix} \mu^2 + 3(k_1 + k_3) + 4k_2 & -2k_1 \\ -2k_1 & \mu^2 + 3(k_1 + k_3) + 4k_2 \end{pmatrix} \quad (2.4)
 \end{aligned}$$

$$\mathbf{A}(2) = \begin{pmatrix} -k_2 & 0 & -k_2 & -k_3 \\ -k_1 & -k_2 & -2k_3 & -k_2 \\ -k_2 & -k_3 & -k_2 & 0 \\ -2k_3 & -k_2 & -k_1 & -k_2 \end{pmatrix} \quad \mathbf{B}(2) = \begin{pmatrix} \rho & -k_1 & -2k_2 & -k_1 \\ -k_1 & \rho & -k_1 & -2k_2 \\ -2k_2 & -k_1 & \rho & -k_1 \\ -k_1 & -2k_2 & -k_1 & \rho \end{pmatrix} \quad (2.5)$$

with

$$\rho = \mu^2 + 3(k_1 + k_3) + 6k_2. \quad (2.6)$$

From $P_m = 3$ upwards, the orders of $\mathbf{A}(P_m)$ and $\mathbf{B}(P_m)$ become increasingly large so that it becomes convenient to express the matrices $\mathbf{A}(P_m)$ and $\mathbf{B}(P_m)$ in block form. Expressing these matrices as $P_m \times P_m$ matrices whose elements are 2×2 submatrices,

Table 1. Matrices for the atomic positions and the configuration σ .

$\mathbf{U}_n(P_m) = \begin{bmatrix} q_{n,0,1} \\ q_{n,0,2} \\ q_{n,1,1} \\ \vdots \\ q_{n,P_m-2,2} \\ q_{n,P_m-1,1} \\ q_{n,P_m-1,2} \end{bmatrix}$	$\mathbf{D}_n(P_m) = \varepsilon \mu^2$	$\begin{bmatrix} \sigma_{n,0,1} \\ \sigma_{n,0,2} \\ \sigma_{n,1,1} \\ \vdots \\ \sigma_{n,P_m-2,2} \\ \sigma_{n,P_m-1,1} \\ \sigma_{n,P_m-1,2} \end{bmatrix}$	$\mathbf{V}(P_n, P_m) = \begin{bmatrix} \mathbf{U}_0(P_m) \\ \mathbf{U}_1(P_m) \\ \mathbf{U}_2(P_m) \\ \vdots \\ \mathbf{U}_{P_n-3}(P_m) \\ \mathbf{U}_{P_n-2}(P_m) \\ \mathbf{U}_{P_n-1}(P_m) \end{bmatrix}$
$\mathbf{F}(P_n, P_m) = \begin{bmatrix} \mathbf{D}_0(P_m) \\ \mathbf{D}_1(P_m) \\ \mathbf{D}_2(P_m) \\ \vdots \\ \mathbf{D}_{P_n-3}(P_m) \\ \mathbf{D}_{P_n-2}(P_m) \\ \mathbf{D}_{P_n-1}(P_m) \end{bmatrix}$	$\psi_j(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \begin{bmatrix} \mathbf{x}_2 & \mathbf{x}_3 & 0 & \dots & 0 & \mathbf{x}_1 \\ \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & 0 & \dots & 0 \\ 0 & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & 0 & \dots & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & \dots & 0 & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & 0 \\ 0 & \dots & 0 & \mathbf{x}_1 & \mathbf{x}_2 & \mathbf{x}_3 & \\ \mathbf{x}_3 & 0 & \dots & 0 & \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$		

we find that they have the same general expression and each of them is determined by a unique set of three 2×2 submatrices, for all $P_m \geq 3$. So we introduce the notation $\psi_j(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ for a matrix $\mathbf{A}(P_m)$ or $\mathbf{B}(P_m)$ associated with the set of 2×2 submatrices $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$, where the subscript j indicates the order of ψ_j (ψ_j is a $j \times j$ matrix). We have introduced this subscript in order to make the ensuing discussion clearer. The general expression of the matrix ψ_j is given in table 1. In this notation the matrices $\mathbf{A}(P_m)$ and $\mathbf{B}(P_m)$ have a simple form; which renders the forthcoming manipulations less cumbersome:

$$\mathbf{A}(P_m) = \psi_{P_m}(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \quad \mathbf{B}(P_m) = \psi_{P_m}(\mathbf{b}_1, \mathbf{b}, \mathbf{b}_1^T) \quad \text{for } P_m \geq 3 \quad (2.7)$$

where

$$\mathbf{a}_1 = \begin{pmatrix} -k_2 & -k_3 \\ -k_3 & -k_2 \end{pmatrix} \quad \mathbf{a}_2 = \begin{pmatrix} -k_2 & 0 \\ -k_1 & -k_2 \end{pmatrix} \quad \mathbf{a}_3 = \begin{pmatrix} 0 & 0 \\ -k_3 & 0 \end{pmatrix} \quad (2.8)$$

$$\mathbf{b}_1 = \begin{pmatrix} -k_2 & -k_1 \\ 0 & -k_2 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} \rho & -k_1 \\ -k_1 & \rho \end{pmatrix}. \quad (2.9)$$

(ii) We now rewrite equation (2.3) with the periodicity condition in the n direction:

$$\mathbf{U}_n(P_m) = \mathbf{U}_{n+P_n}(P_m) \quad (2.10)$$

which gives us a system of P_n matrix equations whose solution is

$$\mathbf{V}(P_n, P_m) = \mathbf{M}(P_n, P_m)^{-1} \mathbf{F}(P_n, P_m). \quad (2.11)$$

In this expression $\mathbf{V}(P_n, P_m)$ and $\mathbf{F}(P_n, P_m)$ are the $2P_n P_m \times 1$ matrices, respectively, for the atomic positions and the configuration σ of a commensurate phase $P_n * P_m$. These matrices are expressed in table 1 as a $P_n \times 1$ matrix whose elements are submatrices

$2P_m \times 1$. $\mathbf{M}(P_n, P_m)$ is a $2P_n P_m \times 2P_n P_m$ matrix characterizing a $P_n * P_m$ phase. This matrix is expressed conveniently as a $P_n \times P_n$ matrix whose elements are submatrices $2P_m \times 2P_m$. Thus, the $1 * P_m$ (quasi-1D structures) and $2 * P_m$ phases are characterized by the following matrices:

$$\mathbf{M}(1, P_m) = \mathbf{A}(P_m) + \mathbf{B}(P_m) + \mathbf{A}(P_m)^T \quad (2.12)$$

$$\mathbf{M}(2, P_m) = \begin{pmatrix} \mathbf{B}(P_m) & \mathbf{A}(P_m) + \mathbf{A}(P_m)^T \\ \mathbf{A}(P_m) + \mathbf{A}(P_m)^T & \mathbf{B}(P_m) \end{pmatrix}. \quad (2.13)$$

From $P_n = 3$ upwards, all the matrices $\mathbf{M}(P_n, P_m)$ have the same general expression as the previous matrix $\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ (table 1), but with $2P_m \times 2P_m$ submatrices as elements. Thus, the notation ψ introduced earlier gives a truly simple expression for higher-period phases:

$$\mathbf{M}(P_n, P_m) = \psi_{P_n}(\mathbf{A}(P_m), \mathbf{B}(P_m), \mathbf{A}(P_m)^T) \quad \text{for } P_n \geq 3. \quad (2.14)$$

Thus, the static solutions $\mathbf{M}(P_n, P_m)$ from which the *atomic positions* for all the commensurate phases of the models are derived are then given by equations (2.12)–(2.14), the $\mathbf{A}(P_m)$ and $\mathbf{B}(P_m)$ being obtained from equations (2.4), (2.5) and (2.7)–(2.9). We see that the matrices $\mathbf{M}(P_n, P_m)$ have a relatively simple expression for all $P_n * P_m$ phases, and we stress that essentially no calculation is required to build up the matrices $\mathbf{M}(P_n, P_m)$, but only elementary *arrangements* of submatrices are necessary. The desired solutions are ultimately obtained by simply working out $\mathbf{M}(P_n, P_m)^{-1}$ in equation (2.11). The procedure is classical and fairly simple. Furthermore, it is also interesting to note from equations (2.7)–(2.9) and (2.14) that, for $P_n * P_m \geq 3 * 3$, all the matrices $\mathbf{M}(P_n, P_m)$ are built up in a straightforward manner from the single set of the 2×2 submatrices $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{b}_1$ and \mathbf{b} . On the other hand we see that the solutions for the lower-period $1 * P_m$ and $2 * P_m$ phases can be entirely calculated analytically from equation (2.11) by elementary *algebraic manipulations* (required to work out $\mathbf{M}(P_n, P_m)^{-1}$) since their corresponding matrices $\mathbf{M}(P_n, P_m)$, respectively, have the simplest expressions (see equations (2.12) and (2.13)). As the periodicity increases, the order of $\mathbf{M}(P_n, P_m)$ becomes increasingly large and so it becomes advantageous to perform equation (2.11) numerically. Furthermore it is very helpful, for determining a PD where a great number of phases have to be examined, to note that all the configurations σ corresponding to the same periodicity $P_n * P_m$ have the same matrix $\mathbf{M}(P_n, P_m)$. Furthermore, the static solutions hence obtained have, of course, to be checked for self-consistency at each site. The self-consistency condition is written as

$$\sigma_{n,m,i} = \text{sgn}(q_{n,m,i}). \quad (2.15)$$

This calculational procedure enables us to study any commensurate phase of the model. Consequently a detailed PD analysis can now be performed, which we illustrate in the following section.

3. Phase diagram

A current problem arises in determining the ground-state (GS) configurations of theoretical lattice models with a double-well substrate potential, owing to the two possible local configurations for each site of the lattice subjected to the double-well potential.

For a given set of the model parameters, the possible periods range from unity (1×1) to infinity ($\infty \times \infty$, i.e. incommensurate phases). Consequently there exists an infinite number of configurations which are candidates for the GS. In general the evaluation of the *absolute (true)* GS is an extremely important problem, for various physical systems. This problem has been solved successfully for some magnetic spin systems using the method of simulated annealing [29–32]. This method can also be used for classical lattice models but necessitates the assumption of some periodicities for the GS [18, 19] because classical theoretical lattices are treated as infinite systems. Usually one assumes a given number of phases of physical interest as candidates for the GS. Very often these are lower-period phases or phases with higher symmetry [1, 7–9, 16–19]. In the present paper we consider only centrosymmetric phases and phases with an inversion centre, because the previous studies of 2D models [1, 16–18] and 1D versions of similar lattices [7–9] show that only these types of phase appear in the PD. As discussed below, phases of physical interest for LiIO_3 have the lowest periodicities, 1×1 and 1×2 . However, we

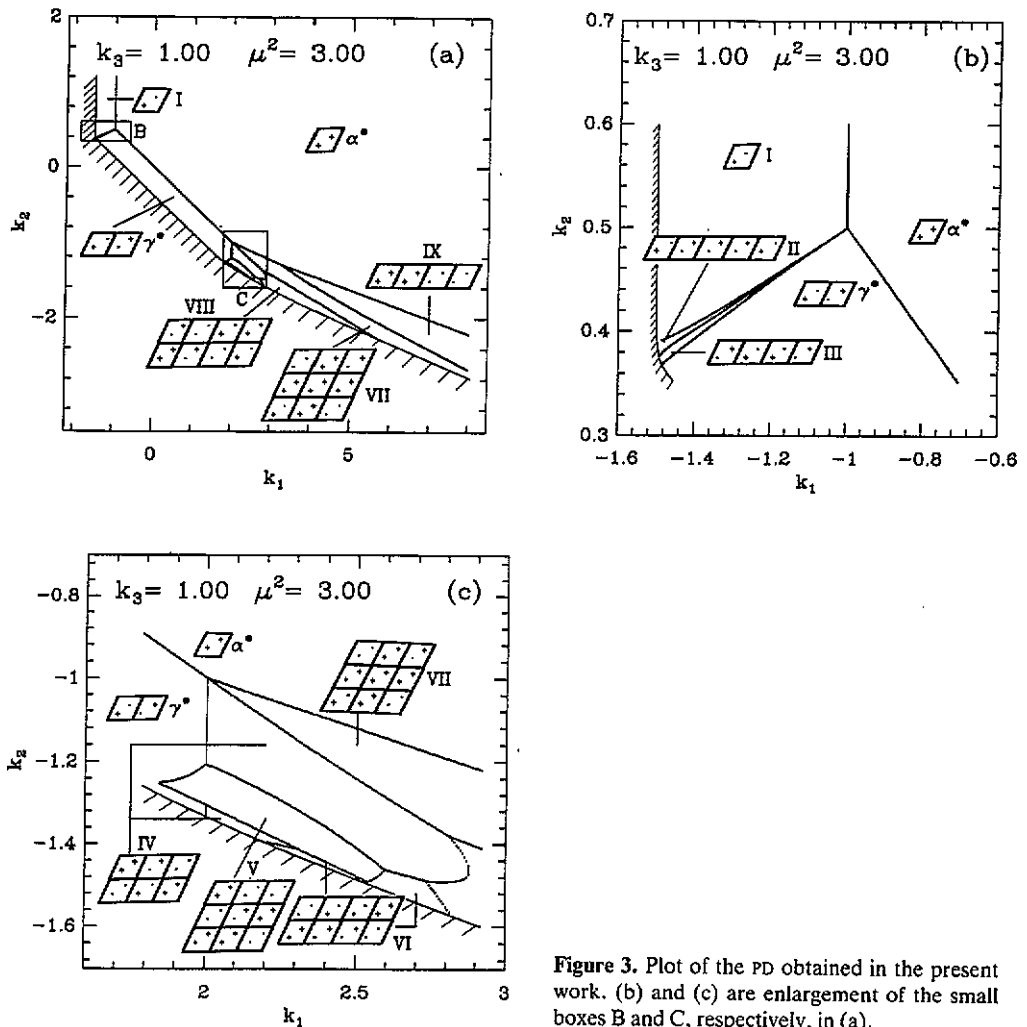


Figure 3. Plot of the PD obtained in the present work. (b) and (c) are enlargement of the small boxes B and C, respectively, in (a).

also include higher-period phases to see whether the *true* 2D phases which do not appear in previous PD (figure 1) can be the GS of the model. We consider the following periodicities: 1×1 , 1×2 , 1×3 , 1×4 , 1×5 , 2×2 , 2×3 , 2×4 and 3×3 . These are sufficient for drawing most of the interesting conclusions for LiIO_3 . There are altogether 512 possible configurations σ corresponding to the above periodicities, but only 140 of them correspond in fact to energetically different phases because of symmetry reasons (these symmetries are discussed in detail in [1]). For a given parameter set, the GS is determined by requiring that the self-consistency condition equation (2.15) is fulfilled and that the phase has the lowest energy of all the investigated phases. We work out numerically equation (2.11), and we consider the same parameter space as in [1] in order to compare our results with that work. We obtain the PD shown in figure 3, where the shaded line indicates the *phonon stability line*. The phonon stability of the model is obtained in detail in [1]. Consequently this point is not discussed in the present paper. In the PD, by α^* and γ^* we denote the 2D *versions* of α - LiIO_3 and γ - LiIO_3 , respectively, obtained by performing a 2D projection of the structure of LiIO_3 onto the a - b plane orthogonal to the c axis of the crystal, as schematically indicated in figure 4 where the angle θ represents the rotational position of an IO_3^- ion. The α -to- γ transition of LiIO_3 is mainly characterized by rotations around the c axis of some IO_3^- ions [20, 21] so that it can be described by the model under consideration. However, it should be mentioned that a quantitative picture of the α -to- γ transition cannot be obtained with the present model because additional theoretical and experimental investigations are required to determine the model parameters, and only a qualitative description can be derived.

We see effectively that in the parameter region $k_1 < 2$, the transition α^* -to- γ^* appears in both the PD derived in the present paper (figure 3) and that obtained in [1] (figure 1), for the same parameter sets k_1 , k_2 ; our PD thus preserves the main result obtained in [1]. We also see that the parameter region for phase I is essentially the same for the two diagrams. These results demonstrate the validity of our calculational procedure for the static solutions presented in section 2. In the other parameter regions the two diagrams are different because of the higher-period phrases that we have included in our investigations. In an effort to clarify the situation, we discuss in the following section the new features of the model which are elucidated by our PD when comparisons with the previous work are made. Furthermore we mention that in figure 1 we have changed the notation used in [1] and used the same notation as for figure 3 just to make the comparison between the two diagrams clearer.

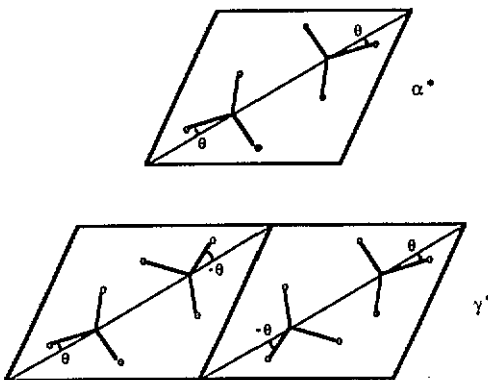


Figure 4. Projection on the a - b plane of the α - and γ -phases of LiIO_3 , denoted α^* and γ^* , respectively.

4. Comparison with other work and discussion

The 2D version of β -LiIO₃ which may have the configuration



(denoted III in [1] is denoted β^* in the present paper. Coquet *et al* [1] noticed that the present model cannot provide a complete description of β -LiIO₃ because the transition γ -to- β also involves rotations of the IO₃⁻ ions around axes lying in the a - b plane (figure 4). However, as β^* appears as a GS in their PD (see figure 1), they then concluded that the present model gives a partial account of β -LiIO₃; this statement is incorrect because our PD (figure 3) shows that β^* is no longer a GS when higher-period phases are included in the investigations. Thus, our PD shows clearly that the 2D hexagonal model under consideration cannot even partially provide a description of the β -phase or the γ -to- β transition of LiIO₃. Consequently, the rotations around the c axis of the crystal of the IO₃⁻ ions are not the preponderant phenomenon of the γ -to- β transition of LiIO₃.

Our PD (figure 3) also shows a great variety of *true* 2D phases, unlike the previous PD (figure 1). These are phases IV, V, VI, VII and VIII. Some quasi-1D phases also appear: these are phases I, II and III. Note that phases II and III do not appear in the previous PD (figure 1). We use the roman numerals to specify that the 3D versions of such phases have never been observed *experimentally* in LiIO₃. The fact that they appear as a GS of this theoretical model does not guarantee that they exist.

In order to determine the parameter region in which the α -to- γ transition of LiIO₃ is qualitatively obtained, Coquet *et al* [1] remarked that, for large k_1 , the α^* -to- γ^* transition disappears, which puts an upper bound on the interesting values of k_1 for LiIO₃, i.e. $k_1 \leq k_{1\max}$. For the latter, $k_{1\max} = 3$ (see figure 1) whereas, for our PD, $k_{1\max} = 2$. We show in a forthcoming paper, where we examine the effects of size on phase transitions, that the α -to- γ transition of LiIO₃ is qualitatively obtained in a small parameter region neighbouring the set $k_1 = -2k_2 = 2$, $\mu^2 = 3k_3 = 1$.

On the other hand, our PD exhibits a special feature of the model, i.e. a re-entrant behaviour which occurs in some parameter regions, with a re-entrant *true* 2D phase. In effect we point out that, when k_2 varies from the border of the phonon stability region towards the α^* -phase region, for $k_1 = 2.1$ (for instance), the system undergoes a transition from phase IV to phase V, and then reverts back to phase IV (see figure 3(c)). Phase V is therefore a re-entrant phase. This unusual phenomenon, called 're-entrant behaviour', has been observed for nematic and smectic phases of some liquid crystalline materials with cyano derivatives [25-27], such as the octyloxybenzoyloxycyano stilbene [25]. Sigaud *et al* [27] have performed a systematic comparative study of several series of chemically neighbouring compounds apt to show a re-entrant behaviour. Coulon and Prost [28] have shown that a quasi-1D system described by two coupled Ising order parameters can show a re-entrant behaviour. The system considered by the latter admits a high-temperature phase and two condensed states as stable phases, and the high-temperature phase is recovered when the two order parameters have the same 'tendency' for condensation [28] which results, according to the latter, from large fluctuations from one condensed state to the other. However, to our knowledge, this interesting phenomenon has not yet been revealed for the 2D non-linear models considered so far. Thus, our results show that a re-entrant behaviour can also occur in a classical 2D non-linear model, with a re-entrant *true* 2D phase (phase V). This is the main result of our paper. Furthermore it should be mentioned that the fact that the re-entrant behaviour

is observed in the model under consideration does not imply that such a phenomenon exists in LiIO_3 . It should be noted that this phenomenon involves a re-entrant phase (phase V) whose 3D version has never been observed experimentally in LiIO_3 . We now summarize all the results of the present paper.

5. Summary and conclusions

We have set up a simple calculational procedure for obtaining the static solutions of atomic positions for all the commensurate phases of a 2D non-linear lattice, considered recently by Coquet *et al* [1] for its interest for LiIO_3 . In the approach developed in the present paper, each commensurate phase $P_n * P_m$ with configuration σ is characterized by a matrix $\mathbf{M}(P_n, P_m)$ from which the static solutions are derived in a straightforward manner by elementary calculations (equation (2.11)). This calculational procedure enables us to investigate any commensurate of the model unlike previous studies of 2D models [1, 11, 16–19]. Throughout the paper, although we have always treated the model in relationship with LiIO_3 (from which the model has been constructed [1]) and focused our attention on its interest for LiIO_3 , we stress that this calculational procedure is quite general and can be easily extended to some other 2D models with a double-quadratic substrate potential such as the triangular lattice examined in [17] or the quadratic lattice considered by Behnke and Büttner [16].

We have derived a more detailed PD than that in previous work [1], which exhibits some new features of the model (figure 3). As general results, we find that the model admits a great variety of true 2D phases as GS (whose 3D versions have never been observed experimentally in LiIO_3). The 2D version of $\beta\text{-LiIO}_3$ (β^*) does not appear in our PD (unlike the previous PD), which means that the rotations around the c axis of LiIO_3 of the IO_3^- ions (i.e. the atomic positions considered in [1] and also in the present paper) are not the preponderant phenomenon of the γ -to- β transition of LiIO_3 . Consequently, the 2D hexagonal model under consideration cannot even partially provide, as claimed in [1], a description of the β -phase or the γ -to- β transition of LiIO_3 . Such a description requires consideration of a 3D model which also includes the rotations of the IO_3^- ions around the axes lying in the a - b plane (figure 4). Furthermore, our PD exhibits an unusual phenomenon, i.e. a re-entrant behaviour with a re-entrant true 2D phase (phase V in figure 3).

All results of the present paper are also of a great interest for some useful extensions of the model, such as the study of the finite versions of the lattice in order to derive the effects of size on phase transitions, which we shall illustrate in a forthcoming paper [33], as it requires that the static structures of the infinite version of the lattice are known.

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