Periodic structures in a two-dimensional lattice

1982 J. Phys. A: Math. Gen. 15 3869

(http://iopscience.iop.org/0305-4470/15/12/035)

J. Phys. A: Math. Gen. **15** (1982) 3869–3875. Printed in Great Britain

Periodic structures in a two-dimensional lattice

G Behnke† and H Büttner‡

† Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80, FRG
‡ Physikalisches Institut, Universität Bayreuth, D-8580 Bayreuth, FRG

Received 7 June 1982

Abstract. A two-dimensional lattice with harmonic interactions to nearest and next-nearest neighbours is studied in detail. The local anharmonic ion–electron interaction is described by a double-quadratic potential. The ground state is a periodic structure with different periods for variable parameters. In a simple mean-field approximation it is found that with changing temperature, transitions between different periodic structures are possible.

1. Introduction

Recently the relation of nonlinear lattices and structural phase transitions has found a growing interest in the literature (Bilz *et al* 1980, 1982, Büttner and Bilz 1981, Büttner 1982, Janssen and Tjon 1981a, b, Axel and Aubry 1981). Since most of the models studied so far have been one-dimensional lattices (with the exception of Bilz *et al* (1982)), it is of great interest to extend the discussion to two-dimensional systems. In this paper a two-dimensional quadratic lattice with polarisable ions is studied in detail. The polarisability is described by a local anharmonic electron–ion coupling. Besides this local anharmonicity there are harmonic nearest and next-nearest neighbour couplings. As in Axel and Aubry (1981) the double-quadratic potential is used to describe anharmonic effects. This double-quadratic potential has been discussed extensively in the literature (see e.g. Trullinger and de Leonardis 1979, Trullinger 1980, Horovitz *et al* 1977, Behnke and Büttner 1981, Peyrard 1981). The main advantage of this potential is that many of the mathematical problems can be solved analytically. The main difference from the ϕ^4 potential is the behaviour for large displacements.

In the present work we will study commensurable static solutions in a quadratic lattice, and compare them with the one-dimensional results of Axel and Aubry (1981). Furthermore, the stability of the various periodic states is discussed in detail. A brief discussion of a mean-field approximation for finite temperatures is included.

2. A two-dimensional shell model

The elements of the lattice are polarisable ions with an ionic core and an electronic shell. The interaction between the core and the shell is described by a double-quadratic potential. The physical ideas behind the shell model are discussed extensively in the literature (see e.g. Büttner and Bilz 1981, Bilz *et al* 1982). The coupling to nearest

0305-4470/82/123869+07$02.00

and next-nearest neighbours is described by harmonic forces. The force constants are denoted by f' and k. The coupling is the same in the x and y direction. Further, we use a diagonal coupling described by f_3. In addition to these ionic couplings we have a shell–shell interaction denoted by f_1. The details of our model can be seen in figure 1. As we can see from Axel and Aubry (1981), we need a competing interaction to nearest and next-nearest neighbours in order to get different ground states for the one-dimensional model. It will be shown that the same is true for our two-dimensional system.

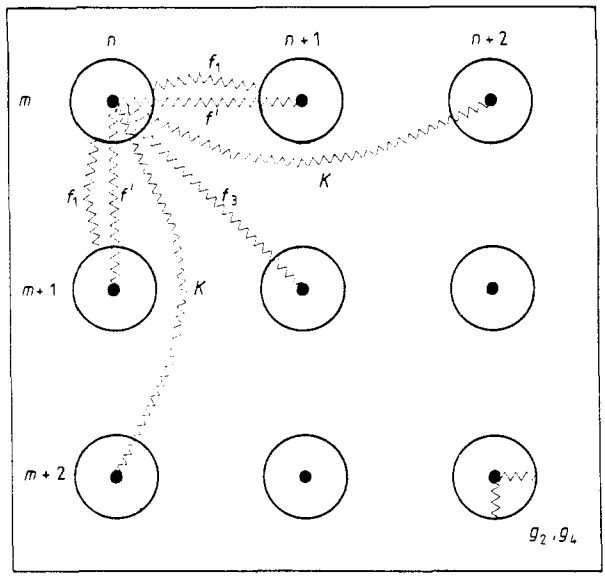

Figure 1. Part of the two-dimensional, quadratic lattice with nearest neighbour harmonic force constants f', next-nearest neighbour constants K in x and y direction and diagonal harmonic force constants f_3 between the ion cores; f_1 is the coupling between the electron shells; the ion core electron–shell coupling is described by a harmonic force constant g_2 and an anharmonic part g_4.

The displacements of the ions are denoted by $\boldsymbol{u}^{mn}$ and those of the electronic shells by $\boldsymbol{v}^{mn}$, with components u_1^{mn}, u_2^{mn} and v_1^{mn}, v_2^{mn}. The corresponding Hamiltonian for this lattice is given by

$$\begin{aligned} H = \tfrac{1}{2}\sum_{m,n}[M(\dot{\boldsymbol{u}}^{mn})^2 + M_e(\dot{\boldsymbol{v}}^{mn})^2] + \tfrac{1}{2}\sum_{m,n}[\![f_1(v_1^{mn} - v_1^{m\,n-1})^2 + f_1(v_2^{mn} - v_2^{m-1\,n})^2 \\ + f'(u_1^{mn} - u_1^{m\,n-1})^2 + f'(u_2^{mn} - u_2^{m-1\,n})^2 + k(u_1^{mn} - u_1^{m\,n-2})^2 \\ + k(u_2^{mn} - u_2^{m-2\,n})^2 + f_3/2\{[(u_1^{mn} - u_1^{m-1\,n-1}) - (u_2^{mn} - u_2^{m-1\,n-1})]^2 \\ + [(u_1^{mn} - u_1^{m+1\,n-1}) + (u_2^{mn} - u_2^{m+1\,n-1})]^2\} + g_2(w_1^{mn})^2 + g_2(w_2^{mn})^2 \\ + g_4[(|w_1^{mn}| - 1)^2 - 1] + g_4[(|w_2^{mn}| - 1)^2 - 1]]\!]. \end{aligned} \tag{1}$$

It should be noted here that the double-quadratic potential can be interpreted as an approximation to the ϕ^4 model (Axel and Aubry 1981) for not too large displacements, since we expect from a physical point of view a strong anharmonicity for large

displacements. In our analytical treatment we prefer the approximate potential, although it may have some disadvantages in the description of real physical systems.

3. The static solutions

We are firstly interested in the possible ground states for zero temperature. They are complicated functions of the various force constants. They are solutions of the following four static coupled nonlinear difference equations:

$$\begin{aligned} M\ddot{u}_1^{mn} = 0 = {} & g_2 z_1^{mn} + f'(u_1^{mn+1} + u_1^{mn-1} - 2u_1^{mn}) + k(u_1^{mn+2} + u_1^{mn-2} - 2u_1^{mn}) \\ & + f_3/2(u_1^{m-1n+1} + u_1^{m+1n-1} + u_1^{m+1n+1} + u_1^{m-1n-1} - 4u_1^{mn} + u_2^{m-1n+1} \\ & + u_2^{m+1n-1} - u_2^{m+1n+1} - u_2^{m-1n-1}), \end{aligned} \tag{2}$$

$$M_e\ddot{v}_1^{mn} = 0 = -g_2 z_1^{mn} + f_1(v_1^{mn+1} + v_1^{mn-1} - 2v_1^{mn}), \tag{3}$$

$$\begin{aligned} M\ddot{u}_2^{mn} = 0 = {} & g_2 z_2^{mn} + f'(u_2^{m+1n} + u_2^{m-1n} - 2u_2^{mn}) + k(u_2^{m+2n} + u_2^{m-2n} - 2u_2^{mn}) \\ & + f_3/2(u_2^{m-1n+1} + u_2^{m+1n-1} + u_2^{m+1n+1} + u_2^{m-1n-1} - 4u_2^{mn} + u_1^{m-1n+1} \\ & + u_1^{m+1n-1} - u_1^{m+1n+1} - u_1^{m-1n-1}), \end{aligned} \tag{4}$$

$$M_e\ddot{v}_2^{mn} = 0 = -g_2 z_2^{mn} + f_1(v_2^{m+1n} + v_2^{m-1n} - 2v_2^{mn}), \tag{5}$$

where the anharmonicities are contained in the abbreviation

$$g_2 z_i^{mn} = g w_i^{mn} - g_4 \operatorname{sgn}(w_i^{mn}) \tag{6}$$

with $g = g_2 + g_4$, and with the difference coordinate $w_i^{mn} = v_i^{mn} - u_i^{mn}$, $i = 1, 2$.

The number of solutions to these equations is quite large and we discuss only commensurable states. Even then there are five different kinds of solutions.

(i) Both displacements u and v are only functions of n. They are the same for all chains.

(ii) The displacements depend only on m and they are the same for all rows n. These solutions are degenerate in energy to those from (i).

(iii, iv) The x components are functions of n (or m) and the y components are functions of m (or n).

(v) The displacements are functions of $(n+m)$. This is the quasi-one-dimensional case.

Explicit calculations show that for the different cases there exist many periodic structures of which some are given in table 1. The functional dependence on the parameters is always the same if one uses an effective ratio

$$a_\nu = g/f_\nu = g(1/f_1 + 1/F_\nu), \qquad \nu = \text{(i)}, \text{(ii)}, \ldots, \text{(v)}, \tag{7}$$

which is different for the cases (i)–(v). The corresponding effective spring constants F_ν are also given in table 1.

The important point is that these periodic structures are not solutions for arbitrary a_ν. While for positive a_ν the structures always exist, we have certain restrictions for negative a_ν. It turns out that the symmetric structures have a lower energy than the asymmetric ones. These symmetric solutions can be written as

$$w_i^{mn} = \pm\alpha w_0 \operatorname{sgn}[\cos(aqp + \phi)] \pm \beta w_0 \cos(aqp + \phi), \qquad i = 1, 2, \tag{8}$$

Table 1. Periodic structures of equations (2)–(5). The force constants F_ν, used in equation (7), are given explicitly for the solutions of the cases (i)–(v).

Period	Structure	$F_{(i)}; F_{(ii)}; F_{(iii)}$	$F_{(iv)}$	$F_{(v)}$	Restrictions
1	↑↑↑	—	—	—	—
2	↑↓	$f'+f_3$	f_3	f'	$a_\nu<-4$
3	×↑↓				
3	↑↓↓	$f'+f_3+k$	f_3+k	$f'+k$	$a_\nu<-3$
4	×↑×↓				$a_\nu<-2$
4	↑↑↓↓	$f'+f_3+2k$	f_3+2k	$f'+2k$	$a_\nu<-2$
4	↑↓↓↓				$a_\nu<-4$
6	×↑↑×↓↓				$a_\nu<-1$
6	↑↑↑↓↓↓	$f'+f_3+3k$	f_3+3k	$f'+3k$	$-3<a_\nu<-1;\ a_\nu<-5$
6	↑↑↓↓↓↓				$a_\nu<-(3+\sqrt{2})$
6	↑↑↓↑↓↓				$a_\nu<-(2+\sqrt{3})$

with $p=n$, m or $(m+n)$; $w_0=g_4/g$, where the phases ϕ depend on the period q. The amplitudes α and β depend only on a_ν. In table 2 we give these parameters for the first symmetric periodic structures. The displacements $\boldsymbol{u}^{mn}$ and $\boldsymbol{v}^{mn}$ are given by similar expressions.

Table 2. Symmetric periodic solutions, given by equation (8).

Structure	aq	ϕ	α	β
↑↑↑	2π	0	0	1
↑↓	π	0	0	$a_\nu/(4+a_\nu)$
×↑↓	$2\pi/3$	$-\pi/2$	0	$(2/\sqrt{3})a_\nu/(3+a_\nu)$
↑↓↓	$2\pi/3$	$-2\pi/3$	1	$-4/(3+a_\nu)$
×↑×↓	$\pi/2$	$-\pi$	0	$a_\nu/(2+a_\nu)$
↑↑↓↓	$\pi/2$	$-3\pi/4$	0	$\sqrt{2}a_\nu/(2+a_\nu)$
×↑↑×↓↓	$\pi/3$	$-\pi/2$	0	$(2/\sqrt{3})a_\nu/(1+a_\nu)$
↑↑↑↓↓↓	$\pi/3$	$-2\pi/3$	$a_\nu/(4+a_\nu)$	$4a_\nu/[(a_\nu+4)(a_\nu+1)]$

The results for the energy calculations can be summarised as follows. For positive coupling constants f', f_1, k and f_3 the solution with period 1 (the ferroelectric state) has always the lowest energy. For negative a_ν we find a variety of possible ground states depending on the coupling constants. The energy for the cases (i) and (ii) is always higher than for (iii, iv) and (v). For these latter cases we give the results in figure 2, where the energy per particle is plotted in units of the ferroelectric ground state energy as a function of a_ν.

For $a_\nu<-4$ the state of period 2 is the ground state. For a_ν between -3 and -4 the state of period 3 is the lowest in energy, and so on (see figure 2). Having calculated these different states and their energy, it is important to know whether these states are really stable with respect to small time-dependent perturbations. We therefore consider small time-dependent disturbances $\boldsymbol{\varepsilon}^{mn}(t)$ to the static solutions and linearise the equations of motion with respect to these perturbations. With the ansatz $\boldsymbol{\varepsilon}^{mn}(t)=$

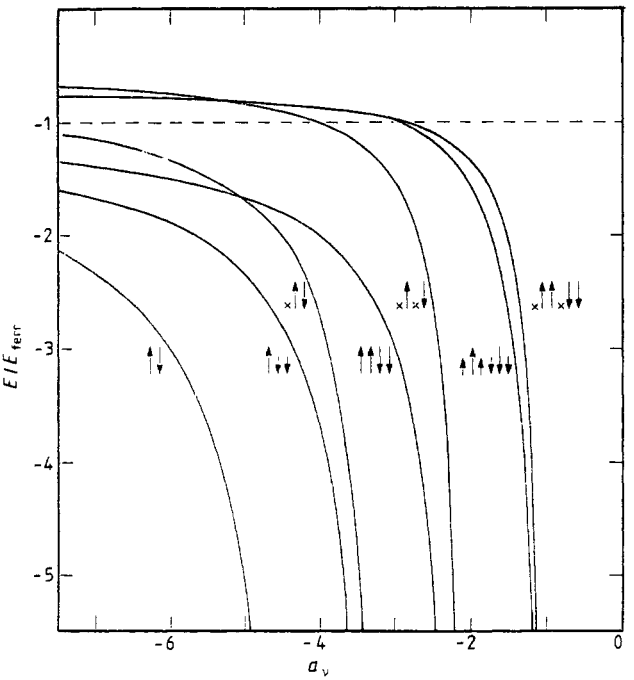

Figure 2. The energy per particle in units of the ferroelectric energy as a function of a_ν for negative force constants for the static solutions of periods 1 to 6.

$\varepsilon_0^{mn} e^{i\omega t}$ one determines the eigenvalue spectrum. The resulting spectrum of these linear equations has to be positive for arbitrary wavenumbers in order to have stable solutions.

The ferroelectric state is found to be stable for positive coupling constants.

The period-2 solution has the spectrum

$$M\omega^2 = [g + 2f_1(1 \mp |\cos qa|)]^{-1}\{2f_1 f'(\cos 2qa \mp |\cos qa|) + 2(1 \mp |\cos qa|)[g(f' + f_1) + 3f_1 f']\} \tag{9}$$

and as a result we find that for $a_\nu < -4$ the solution is stable. In figure 3 we have plotted the dispersion relation for two values of the parameter a_ν. The dispersion of the period-3 solution cannot be given analytically. Numerical studies, however, show that for $-3 > a_\nu > -4$ the states are stable if $f_1 > 0$ and f'/k is of the same order as g/f_1. In figure 4 we give an example for a special set of parameters.

4. Discussion

The periodic structures studied so far describe a large number of possible ground states (for appropriate parameters) at the temperature $T = 0$. The solutions have a similar form to those of the one-dimensional model of Axel and Aubry (1981) (although they seem to have a misprint in their formula (40), where a phase is missing). In contrast to their method, however, our stability analysis tests the dynamic behaviour of the lattice under small perturbations. There are also incommensurable phases, but we are here concerned only with the periodic structures.

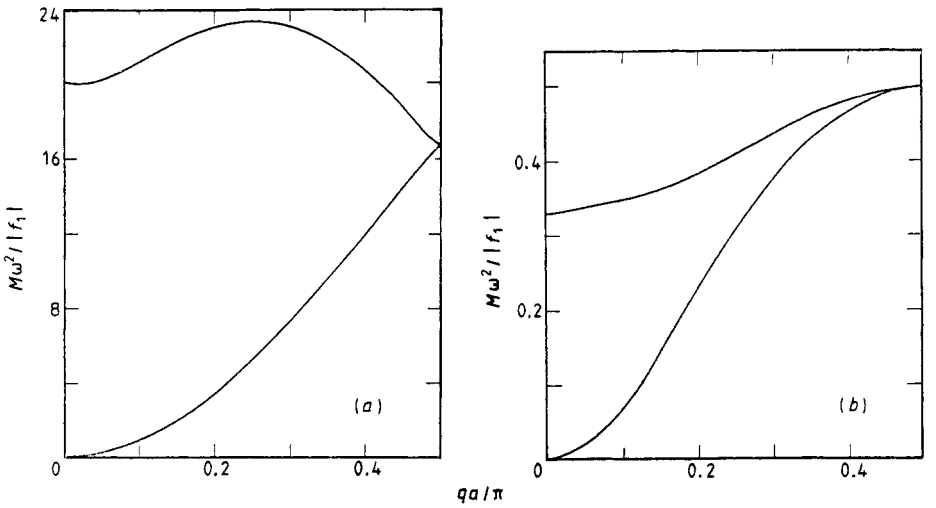

Figure 3. Frequency $M\omega^2$ of the eigenmodes for the perturbation of the period-2 solution as a function of the wavenumber q for two parameter sets: (a), $f_1<0$, $a_\nu=-4.5$; (b), $f_1>0$, $a_\nu=-6$.

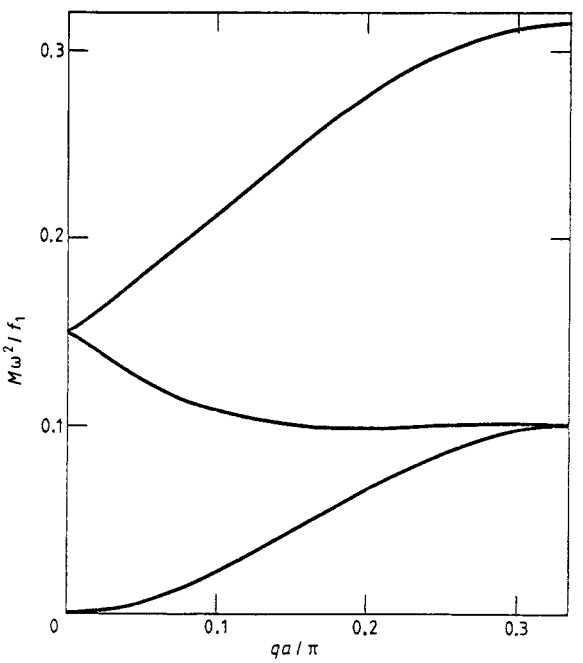

Figure 4. Frequency $M\omega^2$ of the eigenmodes for the perturbation of the period-3 solution '↑↓↓' as a function of the wavenumber q for $g/f_1=3$, $F_\nu/f_1=-0.45$ ($a_\nu=-3.67$).

Finally, we indicate how the possible phase transitions could be studied in a simple mean-field approximation. The method has already been discussed by Janssen and Tjon (1981a, b) for a one-dimensional lattice with non-local anharmonic couplings. Within this approximation it can be shown that effective interaction parameters lead

to different ground states at various temperatures. Instead of discussing the double-quadratic potential we use here the ϕ^4 model, where most of the commensurable states can also be found. It turns out that the harmonic coupling g_2 has to be replaced by

$$g_2 + [\langle (w^{mn})^2 \rangle - \langle w^{mn} \rangle^2] = \tilde{g}_2(T). \tag{10}$$

The thermal fluctuations of the electron–ion displacement increase with increasing temperature, so that the effective coupling $\tilde{g}_2$ is also increasing. Correspondingly we have a change in the parameter ratio a_ν (see equation (7)). In the interesting case of negative force constants, the absolute value of a_ν will increase with increasing temperature. For example, starting with a value for a_ν less than 1, the period-6 solution is the ground state. With increasing temperature solutions of period 4, 3 or 2 become the ground states. Summarising, as the value of a_ν changes, different periodic structures become the energetically favourable configurations of the lattice.

Acknowledgment

The authors would like to thank Professor H Bilz for interesting and stimulating discussions, and Dr N Theodorakopoulus for a critical reading of the manuscript.

References

Axel F and Aubry S 1981 *J. Phys. C: Solid State Phys.* **14** 5433–51
Behnke G and Büttner H 1981 *J. Phys. A: Math. Gen.* **14** L113–6
Bilz H, Bussmann A, Benedek G, Büttner H and Strauch D 1980 *Ferroelectrics* **25** 339–42
Bilz H, Büttner H, Bussmann-Holder A, Kress W and Schröder U 1982 *Phys. Rev. Lett.* **48** 264–7
Büttner H 1982 in *Nonlinear Phenomena at Phase Transitions and Instabilities* ed T Riste (New York: Plenum) p 81
Büttner H and Bilz H 1981 *J. Physique, Colloque* C **6** 111–8
Horovitz B, Krumhansl J A and Domany E 1977 *Phys. Rev. Lett.* **38** 778–81
Janssen T and Tjon J A 1981a *Preprint, Microscopic model for incommensurate crystal phases*
—— 1981b *Phys. Rev.* B **24** 2245–8
Peyrard M 1981 *J. Math. Phys.* **22** 2986–95
Trullinger S E 1980 *J. Math. Phys.* **21** 592–8
Trullinger S E and de Leonardis R M 1979 *Phys. Rev.* A **20** 2225–34