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LETTER TO THE EDITOR

Solitary waves in a two-dimensional diatomic lattice

G Behnke and H Büttner

Physikalisches Institut, Universität Bayreuth, 8580 Bayreuth, West Germany

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Abstract. Static solitary excitations in a two-dimensional diatomic lattice are studied in detail. Our model uses a local anharmonic electron–ion coupling for the polarisability of the anion and harmonic couplings between different chains. This lattice may serve as a model for certain ferro-electric materials. Solitary finite-energy excitations are found and proved to be stable.

Recently the possibility of describing nonlinear structures by solitary-wave excitations has found great interest in condensed matter physics (Behnke 1980, Bishop and Schneider 1978, Horovitz *et al* 1977, Krumhansl and Schrieffer 1975, Schneider and Stoll 1976, Trullinger and de Leonardis 1979, Trullinger 1980). So far most of the models have been one-dimensional lattices with local anharmonic potentials. To our knowledge there is only one two-dimensional example with a special inter-chain coupling where solitary solutions of finite energy have been studied (Horovitz *et al* 1977). It is the aim of this work to study, for the first time, static solutions for a general two-dimensional diatomic lattice which may serve as a model for certain ferro-electrics. It will be shown that this lattice gives a physical interpretation to the model proposed by Horovitz *et al* (1977). Our model starts with the physical observation that in many ferro-electrics a strong and anharmonic polarisability of the anion determines the corresponding lattice dynamics (Bilz *et al* 1980, Büttner and Bilz 1980, Migoni *et al* 1976, Rytz *et al* 1980, Weber and Büttner 1980). Especially the dynamical properties of ferro-electric perovskites have been successfully described in terms of a strongly anisotropic quartic polarisability of the oxygen ion (Bilz *et al* 1980, Büttner and Bilz 1980, Migoni *et al* 1976, Rytz *et al* 1980).

In our two-dimensional lattice we again start with a highly localised electron–ion coupling for the anions within the chain. The main features of our lattice model can be seen in figure 1. It consists of diatomic chains along the x direction with a local anharmonic electron–ion coupling at one side and a rigid ion at the other. These chains are coupled by harmonic non-central forces f_2 and diagonal central forces f_3 between the polarisable anions. The anharmonic potential between the electron and the ion is assumed to be a double-quadratic potential which has been discussed extensively (see Trullinger and de Leonardis 1979, Trullinger 1980). This potential has a different analytic form compared with the ϕ^4 model, but is quite similar in its physical content (see Trullinger and de Leonardis 1979, Trullinger 1980). It is assumed that it is highly anisotropic so that only the displacements in one direction are considered. The displacements of the ions M_1, M_2 and the electron M_e are denoted by u_1^{mn}, u_2^{mn} and v^{mn}, measured in units of the height B of the potential barrier.

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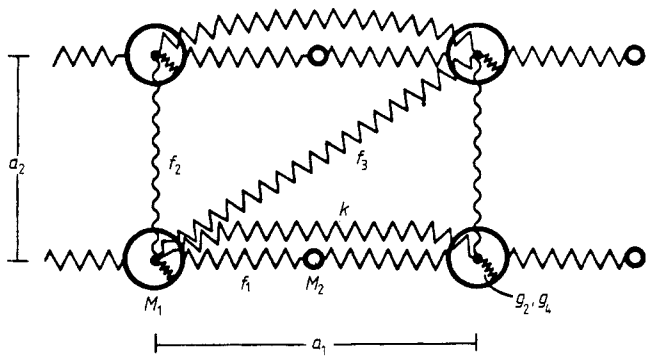

Figure 1. A two-dimensional diatomic lattice for a model ferro-electric with central forces f_1 to nearest neighbours and K to next-nearest neighbours within the chain (x direction); diagonal central forces f_3 and non-central forces f_2 between the anions of different chains (y direction); the ion-core–electron-shell coupling is given by a harmonic force constant g_2 and an anharmonic constant g_4; lattice constants a_1, a_2 and ion masses M_1, M_2.

The Hamiltonian for the lattice shown in figure 1 is written as

$$\begin{aligned} H = \tfrac{1}{2}\sum_{m,n}(M_1(\dot{u}_1^{mn})^2 + M_2(\dot{u}_2^{mn})^2 + M_e(\dot{v}^{mn})^2)B^2 \\ + \tfrac{1}{2}\sum_{m,n}\{f_1(v^{mn}-u_2^{mn})^2 + f_1(v^{mn+1}-u_2^{mn})^2 + K(u_1^{mn}-u_1^{mn+1})^2 \\ + f_2(u_1^{mn}-u_1^{m+1n})^2 + \tfrac{1}{2}\tilde{f}_3[(u_1^{mn}-u_1^{m+1\ n+1})^2 + (u_1^{mn}-u_1^{m+1\ n-1})^2] \\ + g_2(v^{mn}-u_1^{mn})^2 + g_4(|v^{mn}-u_1^{mn}|-1)^2\} \end{aligned} \tag{1}$$

with $\tilde{f}_3 = 2f_3a_1^2/(a_1^2+a_2^2)$, and a_1, a_2 the equilibrium spacings in the x and y directions, respectively. The different chains are enumerated by m, while the different ions in the chain are counted by n. The three resulting equations of motion are coupled nonlinear difference-differential equations. It is assumed that the excitations are only slowly varying in the x direction along the chains. In this case a continuum approximation is appropriate. Within the adiabatic approximation for the electron motion up to second order in a_1 the following equations of motion for $u_1^m(x) = u_1^{mn}$, $u_2^m(x+\frac{1}{2}a_1) = u_2^{mn}$, $v^m(x) = v^{mn}$ result

$$M_1\ddot{u}_1^m = g_2z^m + a_1^2[Ku_1^m + \tfrac{1}{2}\tilde{f}_3(u_1^{m+1}+u_1^{m-1})]_{xx} + (f_2+\tilde{f}_3)(u_1^{m+1}+u_1^{m-1}-2u_1^m) \tag{2}$$

$$M_2\ddot{u}_2^m = f_1[2(v^m-u_2^m) + a_1v_x^m + \tfrac{1}{2}a_1^2v_{xx}^m] \tag{3}$$

$$M_e\ddot{v}^m = 0 = -g_2z^m + f_1[2(u_2^m-v^m) - a_1u_{2_x}^m + \tfrac{1}{2}a_1^2u_{2_{xx}}^m] \tag{4}$$

where the nonlinearity is contained in the abbreviation

$$g_2z^m = (g_2+g_4)(v^m-u_1^m) - g_4\,\mathrm{sgn}(v^m-u_1^m). \tag{5}$$

One should note for the following treatment that $u_2^m(x+\frac{1}{2}a_1)$ has to be expanded for small parameter a_1: $u_2^m(x+\frac{1}{2}a_1) = u_2^m(x) + \frac{1}{2}a_1u_{2_x}^m + \frac{1}{4}a_1^2u_{2_{xx}}^m + \ldots$.

Equations (2)–(4) describe all excitations of our nonlinear two-dimensional diatomic lattice. In the harmonic limit one, of course, obtains the phonon excitations of the lattice. For arbitrary spring constants g_2, K, $\tilde{f}_3$, $f_2 > 0$ and $K > \tilde{f}_3$ the harmonic lattice is found to be stable.

In this work we are mainly interested in static nonlinear solutions of the above equations, that is $\dot{u}_1^m = 0$, $\dot{u}_2^m = 0$. We find the following results.

(i) The ground state is described by a finite relative displacement of the ions (for a negative coupling g_2 with $|g_2| < g_4$):

$$u_1^m = \pm g_4/(g_4 - |g_2|) \qquad v^m = u_2^m = \text{constant}. \tag{6}$$

This solution is similar to that for the ϕ^4 potential. The corresponding ground-state energy is proportional to the number of particles in the lattice and given by $E_g = -ML g_4 |g_2|/2(g_4 - |g_2|)$, where M is the number of chains, each having a length L.

(ii) The phonons above this ground state are identical to the harmonic phonons, if g_2 is replaced by $g_4 - |g_2|$.

(iii) The most interesting solutions, however, are the nonlinear excitations above the ground state. For solving the corresponding equations, it is useful to introduce the difference variable $w^m(x) = v^m(x) - u_1^m(x)$. The most general localised nonlinear excitations above the ground state that are continuous in the x direction and satisfy

$$\operatorname{sgn} w^m = \begin{cases} \operatorname{sgn} x & \text{for } m = 0 \\ 1 & \text{for } m \neq 0 \end{cases} \tag{7}$$

can be written as

$$w_0^m(x) = \begin{cases} (A + I_0(x)) \operatorname{sgn} x & \text{for } m = 0 \\ A + I_m(x) \operatorname{sgn} x & \text{for } m \neq 0 \end{cases} \tag{8}$$

$$u_{1_0}^m(x) = J_m(x) \operatorname{sgn} x \tag{9}$$

$$u_{2_0}^m(x) = w_0^m(x) + u_{1_0}^m(x) \tag{10}$$

with $A = g_4/(g_4 - |g_2|)$.

The quantities $I_m(x)$ and $J_m(x)$ are given explicitly by the following integrals:

$$\begin{aligned} I_m(x) &= \sum_{i=1}^{2} \int_{-\pi}^{\pi} \mathrm{d}q_2/2\pi\, B_i(q_2) \exp(-\alpha_i(q_2)|x|) \\ J_m(x) &= \sum_{i=1}^{2} (-1)^{i+1} \int_{-\pi}^{\pi} \mathrm{d}q_2/2\pi\, A_1(q_2) \exp(-\alpha_i(q_2)|x|). \end{aligned} \tag{11}$$

The wavenumbers $\alpha_{1,2}$ as well as the amplitudes A_1, $B_{1,2}$ are the following functions of q_2:

$$a_1^2 \alpha_{1,2}^2 = [\beta_1 \pm (\beta_1^2 - 4\beta_2)^{1/2}]/[2f_1(K + \tilde{f}_3 \cos q_2)] \tag{12}$$

with

$$\begin{aligned} \beta_1 &= (g_4 - |g_2|)(f_1 + 2(K + \tilde{f}_3 \cos q_2)) + 2f_1(f_2 + \tilde{f}_3)(1 - \cos q_2) \\ \beta_2 &= 4f_1(f_2 + \tilde{f}_3)(g_4 - |g_2|)(K + \tilde{f}_3 \cos q_2)(1 - \cos q_2) \end{aligned} \tag{13}$$

and

$$\begin{aligned} A_1 &= g_4[(K + \tilde{f}_3 \cos q_2) a_1^2 (\alpha_1^2 - \alpha_2^2)]^{-1} \\ B_{1,2} &= \mp A_1 f_1 a_1^2 \alpha_{1,2}^2 [f_1 a_1^2 \alpha_{1,2}^2 - 2(g_4 - |g_2|)]^{-1}. \end{aligned} \tag{14}$$

These solutions are valid for arbitrary lattice parameters g_2, g_4, K, f_2 and $\tilde{f}_3$. The solution for $w^m(x)$ describes a kink excitation in one chain, while the displacements in the neighbouring chains are nearly unaltered. These solutions contain in the limit $f_1 \to \infty$ and $f_2 = -\tilde{f}_3$ those described by Horovitz *et al* (1977). Therefore it is obvious

that the special coupling introduced by Horovitz can be interpreted as a partial compensation of non-central and diagonal forces in the lattice. The solutions for $u_1^m(x)$ are different from $w^m(x)$ slowly oscillating functions for all chains.

(iv) The solutions (8)–(10) are stable against small perturbations. To see this the static solutions are disturbed by small additive functions $\psi_i^m(x, t)$. Using the fact that the static parts are solutions of the equations (2)–(4) and by linearisation with respect to the small perturbations we find three coupled linear difference-differential equations with non-constant coefficients. With the ansatz $\psi_i^m = f_i^m(x)\,e^{i\omega t}$, $i = 1, 2, 3$ one determines the spectrum and finds the corresponding eigenfunctions. There is a single bound state with $\omega = 0$ and various scattering states of odd and even parity with $\omega^2 > 0$. The dispersion relation for ω is equivalent to that of the harmonic lattice by substituting g_2 by $(g_4 - |g_2|)$. Since the potential of the model ferro-electric is such that $|g_2| < g_4$ the dispersion yields, the same as for the harmonic case, positive values for ω^2 for arbitrary lattice constants and $K > \tilde{f}_3$. Therefore we conclude that static excitations (8)–(10) are stable against small perturbations.

(v) Another important feature of the solutions (8)–(10) is that the resulting excitation energy $E_{ex} = E - E_g$ is finite and does not depend on the size of the lattice. Therefore the solutions can be described as solitary excitations of the lattice. The explicit expression for the energy is too lengthy to be reproduced here. As an example we give the results for the following typical lattice parameters, $|g_2|/2f_1 = 0.25$, $g_4/2f_1 = 0.27$, $K/2f_1 = 0.1$, $\tilde{f}_3/2f_1 = f_2/2f_1 = 0.05$. The ground-state energy per particle in units of f_1 is found to be $E_g = 1.69$ and the corresponding excitation energy in units of E_g, $E_{ex} = 7.12$.

Summarising it should be noted that these finite-energy excitations are really static and that the dynamics of our system are much more complicated than in the Horovitz model. There is an interaction between acoustic and optical excitations and therefore the static kink solution will be deformed when it moves through the lattice. More general, stationary solutions to equations (2)–(4) are currently under investigation and their relation to the structure function of the lattice will be studied in detail. Only in the limit of a very large cation mass M_2 and very strong intra-chain coupling f_1 the diatomic lattice reduces to a monatomic chain with local potentials. In this limit simple Lorentz-invariant wave-equations are found from (2)–(4).

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