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Dynamics of a Nonlinear Diatomic Chain

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Abstract

We examine nonlinear lattice excitations in a model for a solid which may undergo a displacive structural phase transition. In particular, we investigate the field equations for a diatomic chain of atoms including nonlinear potentials on one species. We identify three classes of excitations in this model. These are linearized phonons, large amplitude solitary waves, and nonlinear phonons. Interactions between the linear phonons and the nonlinear modes give rise to a translation mode which is a further solution of the field equations. The linear and nonlinear phonons are also direct solutions of the discrete equations of motion. However, using the molecular dynamics technique we find that kink-type configurations occur for a much larger parameter space in the discrete lattice than they do in the continuum description. All the stable excitations of the field equations should be included in a formal description (e.g. statistical mechanics) of the model.

1. Introduction

The study of nonlinear excitations in condensed matter physics is currently a very active field of research (Bishop *et al.* 1980). This is particularly so in systems where perturbation schemes are unsatisfactory due to large amplitude displacements of atoms from equilibrium. Such configurations may be found in models of systems which undergo a structural phase transition (Cowley 1980; Bruce 1980; Bruce and Cowley 1980).

A structural phase transition simply involves a rearrangement of the lattice equilibrium structure at a critical temperature. Macroscopic properties such as specific heat and thermal expansion change at the transition. The 'cluster picture' for these transitions (Schneider and Stoll 1973, 1976; Krumhansl and Schrieffer 1975; Bruce and Cowley 1980) is based on a collection of thermally excited pseudo-particles. In this picture, it is assumed that solids which undergo structural phase transitions typically have a doubly degenerate ground state. At zero temperature the system is in perfect order (one of its ground states). As the temperature is raised the constituent atoms move from their position in perfect order. These imperfections have a characteristic wavelength (excitation energy). Furthermore, it is expected that for weakly disordered systems a superposition of imperfections may constitute another imperfection. Hence the system, when in a low lying state, may be regarded as a collection of elementary excitations (Bishop *et al.* 1980).

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Molecular dynamics studies of a model undergoing a structural phase transition (Schneider and Stoll 1973, 1976) revealed the presence of two distinct types of excitation. These are (i) oscillations of the atoms about their 'equilibrium' positions and (ii) configurations of clusters of atoms in one ground state separated by a 'domain wall' from neighbouring clusters in the other ground state. The first analytic studies to include both types of excitation were the non-perturbative treatments by Aubry (1974), Krumhansl and Schrieffer (1975) and Varma (1976). The Hamiltonian for their microscopic models is described by

$$H = \sum_i \{\tfrac{1}{2}m\dot{u}_i^2 + \tfrac{1}{2}\gamma(u_i - u_{i+1})^2 + V(u_i)\}. \tag{1}$$

This represents a monatomic chain of atoms with linear nearest neighbour forces and an additional single site potential $V(u)$, which is usually taken to have a double well form. The potential $V(u)$ arises from the other atoms in the solid. The system is illustrated in Fig. 1.

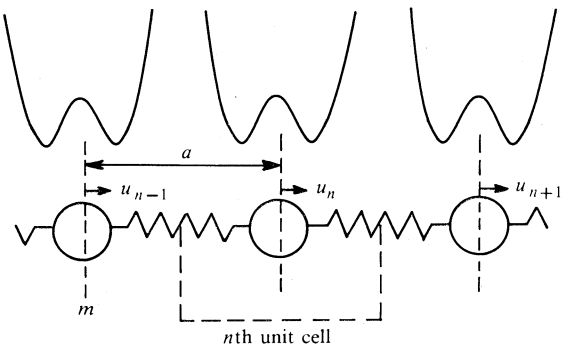

Fig. 1. Standard model for structural phase transitions in solids. This is a monatomic chain of masses m coupled by harmonic interactions of spring constant γ. There is a nonlinear on-site potential on each atom. The length of the unit cell is a.

The Hamiltonian (1) can model two limiting types of structural phase transitions, called order–disorder transitions and displacive transitions (Aubry 1974). The order–disorder regime occurs when the nearest neighbour interaction energy is small compared with the single particle potential barrier energy. In this case the atoms are randomly displaced in one of the bottoms of the double well. At low temperatures where the thermal energy is much less than the barrier energy a pseudo-spin formalism can be applied (Aubry 1974; Bruce 1980) leading to an Ising model description. The displacive regime occurs in the other limit where the intersite coupling is dominant. In this case 'exact' nonlinear techniques become important since, near the transition temperature, displacements may be very large and invalidate perturbation methods. We restrict ourselves to the displacive regime in this paper. Here, the strong coupling means that the displacement field should not alter greatly over a lattice spacing a (i.e. the wavelength of a displacement pattern will be much greater than the lattice constant). This is the basis of the continuum approximation which connects

displacements of neighbouring atoms by a Taylor series. The Hamiltonian (1) in the continuum limit up to second order in a is

$$H \approx \int \frac{\mathrm{d}x}{a} \{\tfrac{1}{2}m\dot{u}^2 + \tfrac{1}{2}\gamma a^2 u'^2 + V(u)\}. \tag{2}$$

Krumhansl and Schrieffer (KS) (1975) investigated the continuum Hamiltonian with the 'ϕ^4' double well potential

$$V(u) = -\tfrac{1}{2}Au^2 + \tfrac{1}{4}Bu^4, \qquad A, B > 0. \tag{3}$$

They found two classes of low temperature solutions to the classical equations of motion. They identified these excitations as phonons, and nonlinear kinks. The kink solution,

$$u = u_0 \tanh\{(x - vt)/\sqrt{2}\,\xi\}, \tag{4}$$

where $u_0 = (A/B)^{\frac{1}{2}}$, transfers the displacement pattern from $-u_0$ to $+u_0$ over a domain wall of thickness $2\sqrt{2}\,\xi$. Using functional integral methods (Scalapino *et al.* 1972), KS were able to exactly calculate the classical partition function for this chain. They found that the free energy decoupled into an oscillating contribution and a tunnelling contribution. The oscillating contribution corresponds to the phonon free energy for vibrations in a well. This led KS to speculate that the tunnelling contribution might correspond to a gas of kinks. Indeed, a calculation of the free energy of the chain at low temperatures, based on a phenomenological model of an ideal gas of completely non-interacting phonons and kinks, yielded good agreement with the 'exact' transfer integral calculation. Even better agreement was obtained by including kink–phonon interactions in the 'ideal gas' model (Currie *et al.* 1980). The model has since been extended to other potentials (Gupta and Sutherland 1976; Trullinger and De Leonardis 1977; Currie *et al.* 1980), higher dimensions (Bishop and Krumhansl 1975), two component field systems (Currie *et al.* 1979; Trullinger and De Leonardis 1980) and to lattices with more than one type of atom (Büttner and Bilz 1978).

In the present paper, we generalize the approach of KS to a diatomic chain. In Section 2 we present the model, derive the coupled field equations of motion and show that in the correct limit one obtains the continuum equations for a harmonic diatomic chain. In Section 3 we derive three classes of solutions of our nonlinear field equations. We identify linearized phonon solutions, equal displacement field solitary waves, and nonlinear periodic solutions. The nonlinear periodic solutions are shown to be the continuum analogue of discrete lattice 'periodon' solutions (Büttner and Bilz 1981). In Section 4 we discuss numerical investigations of our model including some preliminary molecular dynamics results. In Section 5 we make some remarks concerning the possible role of the solutions of our field equations in the statistical mechanics of the diatomic model. We conclude with a summary in Section 6.

2. Diatomic Model for Displacive Phase Transitions

An obvious extension to the model examined by KS is to include two types of atom in the chain, since many of the solids which undergo displacive phase transitions (e.g. $BaTiO_3$) have a diatomic structure in the (100) direction. Most studies of

nonlinear diatomic lattices in this regard have dealt with nonlinear interactions between nearest neighbours (Büttner and Bilz 1978; Yajima and Satsuma 1979; Dash and Patnaik 1981; Pnevmatikos *et al.* 1983). This type of nonlinearity is similar to that considered in original studies of nonlinear monatomic chains (Fermi *et al.* 1965; Zabusky and Kruskal 1965). In the continuum description of these diatomic chains only approximate solutions to the coupled field equations of motion have been attained. Recently, a new nonlinear diatomic model has been presented (Subbaswamy and Mills 1978; Henry *et al.* 1982) in which the nonlinearity is similar to the KS form. Furthermore, exact solutions have been obtained for the equations of motion describing this model in the continuum limit (Henry *et al.* 1982). We note that exact solutions have also recently been reported by Büttner and Bilz (1981) in the continuum and discrete description of a nonlinear diatomic chain.

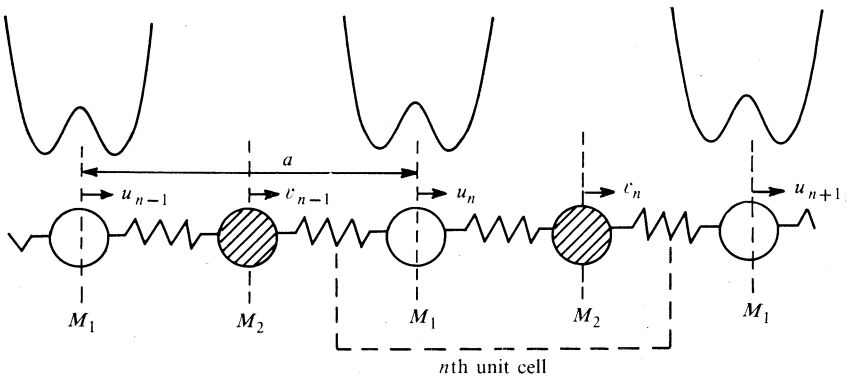

Fig. 2. Present model consisting of a diatomic chain with masses M_1 and M_2. Nearest neighbour masses are coupled by harmonic interactions of spring constant γ. One species, M_1, can occupy one of two off-centre sites. The length of the unit cell is a.

The model we examine consists of a diatomic chain of harmonically coupled nearest neighbour atoms, M_1 and M_2, including a nonlinear potential on one species M_1 (Fig. 2). The Hamiltonian for the discrete lattice is taken to be

$$H = \sum \tfrac{1}{2}M_1 \dot{u}_i^2 + \tfrac{1}{2}M_2 \dot{v}_i^2 + \tfrac{1}{2}\gamma(u_i - v_{i-1})^2 + \tfrac{1}{2}\gamma(u_i - v_i)^2 + V(u_i), \tag{5}$$

where u_i and v_i are the displacements of the two types of atom in the ith unit cell.

The corresponding equations of motion are

$$M_1 \ddot{u}_n = -\gamma(2u_n - v_{n-1} - v_n) - V'(u_n), \tag{6a}$$

$$M_2 \ddot{v}_n = -\gamma(2v_n - u_n - u_{n+1}). \tag{6b}$$

Subbaswamy and Mills (1978) have studied a similar model in connection with order–disorder type structural phase transitions. Here we examine the model Hamiltonian (5) in the displacive regime. Displacive structural phase transitions may occur in this model when the single particle barrier energy $V(u_0)$ (i.e. the energy required to move an atom from the bottom to the top of one of the wells) is smaller than the associated change in the nearest neighbour interaction energy γu_0^2 [assuming all other atoms are in perfect order (Cowley 1980)], i.e.

$$\gamma > |V(u_0)|/u_0^2, \tag{7}$$

where $\pm u_0$ defines the positions of the minima of the double well potential. The relative strength of the coupling constant allows us to employ the continuum approximation in which a Taylor series expansion can be used to connect displacement fields of like atoms in neighbouring unit cells. We thus derive the continuum Hamiltonian in terms of two displacement fields $u(x,t)$ and $v(x,t)$ by making the substitutions (retaining terms only up to second order in a)

$$u_i \to u(x,t) \to u\,,$$

$$v_i \to v(x+\tfrac{1}{2}a,t) \to v+\tfrac{1}{2}av'+\tfrac{1}{2}(\tfrac{1}{2}a)^2v''\,,$$

$$v_{i-1} \to v(x-\tfrac{1}{2}a,t) \to v-\tfrac{1}{2}av'+\tfrac{1}{2}(\tfrac{1}{2}a)^2v''\,,$$

$$\sum_i \to \int \frac{\mathrm{d}x}{a},$$

in the discrete Hamiltonian (5). Omitting total differential terms (which do not contribute to the resulting equations of motion) we arrive at the continuum Hamiltonian

$$H = \int \frac{\mathrm{d}x}{a}\tilde{H} = \int \frac{\mathrm{d}x}{a}\{\tfrac{1}{2}M_1\dot{u}^2+\tfrac{1}{2}M_2\dot{v}^2+\gamma(u-v)^2+\tfrac{1}{4}\gamma a^2u'v'+V(u)\}\,. \tag{8}$$

The coupled field equations of motion which follow from equation (8) are

$$M_1\ddot{u}+2\gamma(u-v)-\tfrac{1}{4}\gamma a^2v''+\partial V/\partial u = 0\,, \tag{9a}$$

$$M_2\ddot{v}+2\gamma(v-u)-\tfrac{1}{4}\gamma a^2u'' = 0\,. \tag{9b}$$

If we set $V = 0$ then equations (9) reduce to the continuum equations of motion for a harmonic diatomic chain. Making the substitutions

$$u = A_1\exp\{\mathrm{i}(kx-\omega t)\}\,, \qquad v = A_2\exp\{\mathrm{i}(kx-\omega t)\}\,,$$

we obtain the dispersion law

$$\omega^2 = \gamma\frac{M_1+M_2}{M_1M_2}\left\{1\pm\left(1-\frac{M_1M_2(a^2k^2-\frac{1}{16}a^4k^4)}{(M_1+M_2)^2}\right)^{\frac{1}{2}}\right\}. \tag{10}$$

This contains the well-known acoustic branch

$$\omega^2 = c_A^2k^2\,, \tag{11}$$

where $c_A^2 = \gamma a^2/2(M_1+M_2)$, and the optic branch

$$\omega^2 = 2(M_1+M_2)/M_1M_2-c_A^2k^2\,, \tag{12}$$

for the harmonic diatomic chain, in the long wavelength limit $ka \ll 1$.

3. Excitations in the Diatomic Chain

In the remainder of this work we include the ϕ^4 nonlinear single site potential (3) in the field equation (8). This allows us the possibility of finding three distinct classes of solution.

(a) Linearized Periodic Solutions

Both low and high energy phonons can be identified in the nonlinear diatomic chain. These types of excitation are configurationally distinct. The low energy phonons represent small oscillations of the M_1 atoms in one of the bottoms of the double well potential [i.e. about $\pm u_0 = \pm(A/B)^{\frac{1}{2}}$], and oscillations of the M_2 atoms about $\pm u_0$ from their equilibrium positions. Explicitly, these low energy linearized phonons are

$$u = \pm u_0 + u_L \sin(kx - \omega_L t + \phi), \qquad u_L \ll 1, \tag{13a}$$

$$v = \pm u_0 + v_L \sin(kx - \omega_L t + \phi), \qquad v_L \ll 1, \tag{13b}$$

with the dispersion relation

$$\omega_L^2(\pm) = \frac{AM_2 + \gamma(M_1+M_2)}{M_1 M_2}\left\{1 \pm \left(1 - \frac{(4A\gamma + \gamma^2 a^2 k^2 - \frac{1}{16}\gamma^2 a^2 k^4) M_1 M_2}{\{AM_2 + \gamma(M_1+M_2)\}^2}\right)^{\frac{1}{2}}\right\}. \tag{14}$$

We note immediately that we cannot simply identify the lower branch of equation (14), $\omega_L^2(-)$, as an acoustic branch [$\omega_L^2(-)|_{k=0} \neq 0$], as is the case in the harmonic diatomic chain. Instead, we consider the long wavelength limit ($ka \ll 1$), in which case the lattice will be highly displacive ($A \ll \gamma$), and we derive

$$\omega_L^2(-) = (\tfrac{1}{2}\gamma^2 a^2 k^2 + 2A\gamma)/\{AM_2 + \gamma(M_1+M_2)\}, \tag{15}$$

$$\omega_L^2(+) = 2\{AM_2 + \gamma(M_1+M_2)\}/M_1 M_2 - \omega_L^2(-). \tag{16}$$

Equation (15) defines $\omega_L^2(-)$ for all $k \geqslant 0$ and reduces to the dispersion relation for low energy phonons in the KS monatomic chain (their equation 14) in the correct limit $M_2 \to 0$. The upper branch (16) for $\omega_L^2(+)$ is only defined for a restricted range of k and is a direct consequence of the diatomic nature of the chain.

High energy phonons represent vibrations of the atoms about their equilibrium positions ($u = v = 0$). In Section 3*c* we show that these vibrations are nonlinear and are an exact solution of the equations of motion.

(b) Solitary Wave Solutions

The preceding linearized periodic solutions are low amplitude solutions. The field equations also support large amplitude solutions. The simplest large amplitude solutions describe a static u field with a static or oscillating v field, i.e.

$$u = \pm u_0, \qquad v = u \pm v_0 \sin(kct + \phi_1)\sin(kx + \phi_2), \tag{17a, b}$$

where $k = (8/a^2)^{\frac{1}{2}}$ and $c = (\gamma a^2/4M_2)^{\frac{1}{2}}$. The particular solution $v = u = \pm u_0$ is the lowest energy (ground state) solution. The energy of this solution is defined as zero and this is taken as the reference level for the other solutions which can be regarded as excitations above this level. The energy level difference

$$E = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{a}\{\tfrac{1}{2}M_1 \dot{u}^2 + \tfrac{1}{2}M_2 \dot{v}^2 + \gamma(u-v)^2 + \tfrac{1}{4}\gamma a^2 u' v' - \tfrac{1}{2}A(u^2 - u_0^2) + \tfrac{1}{4}B(u^4 - u_0^4)\} \tag{18}$$

is the excitation energy of the solution.

A more interesting class of large amplitude solutions is comprised of solitary wave solutions. A solitary wave is defined as a localized travelling wave (Scott *et al.* 1973). Hence, in order to investigate the field equations for solitary wave solutions we make the travelling wave substitutions

$$u(x,t) = f(s), \qquad v(x,t) = g(s), \tag{19a, b}$$

with $s = x - ct$, where c is the speed of the travelling wave in the field equations (9). This gives the set of equations

$$\begin{pmatrix} \frac{1}{4}\gamma a^2 & 2\gamma \\ M_2 c^2 & 2\gamma \end{pmatrix} \begin{pmatrix} \mathrm{d}^2 g/\mathrm{d}s^2 \\ g \end{pmatrix} = \begin{pmatrix} M_1 c^2 (\mathrm{d}^2 f/\mathrm{d}s^2) + 2\gamma f + \partial V/\partial f \\ \frac{1}{4}\gamma a^2 (\mathrm{d}^2 f/\mathrm{d}s^2) + 2\gamma f \end{pmatrix}. \tag{20}$$

For the particular characteristic velocity

$$c = c_0 = (\gamma a^2/4M_2)^{\frac{1}{2}}, \tag{21}$$

the second equation in (20) tells us that the two displacement fields will be 'equal', and the first equation gives us the structure of these fields. Explicitly we have (Henry *et al.* 1982)

$$g(s) = f_0(s); \quad s = \{c_0^2(M_1 - M_2)\}^{\frac{1}{2}} \int^{f_0} \{C - 2V(f)\}^{-\frac{1}{2}} \, \mathrm{d}f. \tag{22}$$

For appropriate choices of the integration constant, equation (22) describes the solitary wave solutions of the corresponding monatomic chains, described by Currie and coworkers (1980) for an entire class of nonlinear potentials (e.g. ϕ^4, sine–Gordon, double quadratic). However, in this case, the Lorentz invariance of the solutions is destroyed (cf. Büttner and Bilz 1981), with the speed of the solitary waves now fixed by the parameters of the problem.

Including the ϕ^4 potential (3) in equation (22) we note the following solitary wave solutions:

(i) For $M_1 < M_2$, $C = 2V(u_0)$ yields the kink solution

$$v(x,t) = u(x,t) = \pm u_0 \tanh(s/\xi_K); \qquad \xi_K = \{A^{-1} 2c_0^2 (M_2 - M_1)\}^{\frac{1}{2}}. \tag{23}$$

(ii) For $M_1 > M_2$, $C = 0$ yields the pulse solution

$$v(x,t) = u(x,t) = \pm\sqrt{2}\, u_0 \operatorname{sech}(s/\xi_P); \quad \xi_P = \{A^{-1} c_0^2 (M_1 - M_2)\}^{\frac{1}{2}}. \tag{24}$$

A more general solution than these equal displacement field, large amplitude solitary waves of equations (23) and (24), includes an oscillating (acoustic phonon) term in the v field. In this case

$$u = u_s(s), \tag{25a}$$

$$v = u + v_0 \sin(ks + \phi); \quad k = (8a^{-2})^{\frac{1}{2}}, \tag{25b}$$

where $u_s(s)$ is one of the solitary wave solutions described above. This tells us that the solitary waves which propagate at $c = c_0$ are unmodified by (i.e. do not interact with) phonons in the v field with wavevector $k = (8a^{-2})^{\frac{1}{2}}$. They do, however, interact with phonons in both fields. The nature of this interaction determines the linear stability of the solutions (see Section 5).

The pulse solution is a non-topological infinite energy solution, whereas the kink solution is topologically stable and of finite energy. A knowledge of the stability and excitation energy of 'nonlinear sectors' of solution space is important in considerations of statistical mechanics (see Section 5).

The equal displacement field kinks (23) are clearly 'acoustic' (in phase) solutions. Hence for a certain characteristic velocity the nonlinear field equations admit strictly acoustic solutions. The characteristic velocity $c = c_0$ of equation (21) is the acoustic velocity for a harmonic chain with $M_1 = M_2$. In other types of nonlinear diatomic lattice models, where the nearest neighbour interactions contain the nonlinearity, acoustic mode solutions have been found using the *ansatz* (Büttner and Bilz 1978; Dash and Patnaik 1981)

$$v(x+\tfrac{1}{2}a) = u(x) + \beta_1 \tfrac{1}{2}a\,u'(x) + \tfrac{1}{2}\beta_2(\tfrac{1}{2}a)^2\,u''(x) + \ldots, \tag{26}$$

where the β_i are general coefficients determined by the parameters of the problem. Our $v(x) = u(x)$ solutions correspond to all $\beta_i = 1$. In diatomic chains with nonlinear nearest neighbour interactions this corresponds to $M_1 = M_2$. In our chain, this clearly does not follow. In both types of diatomic chain, however, the acoustic mode solitary wave solutions are similar to those found in the corresponding monatomic chain except for restrictions on the parameters.

(c) *Nonlinear Periodic Solutions*

For $c \neq c_0$, the displacement fields are not equal and the travelling waves may become extended. In this case the equations of motion (20) may be decoupled in which case a fourth-order nonlinear differential equation for f is derived:

$$\{c^4 M_1 M_2 - (\tfrac{1}{4}\gamma a^2)^2\}\frac{\mathrm{d}^4 f}{\mathrm{d}s^4} + \{2\gamma c^2(M_1+M_2) - \gamma^2 a^2\}\frac{\mathrm{d}^2 f}{\mathrm{d}s^2}$$

$$+ c^2 M_2 \frac{\mathrm{d}^2}{\mathrm{d}s^2}\left(\frac{\partial V}{\partial f}\right) + 2\gamma\frac{\partial V}{\partial f} = 0, \tag{27}$$

with the corresponding solution

$$g = \{c^4 M_1 M_2 - (\tfrac{1}{4}\gamma a^2)^2\}\mathrm{d}^2 f/\mathrm{d}s^2 + f + [c^2 M_2/\{2\gamma(c^2 M_2 - \tfrac{1}{4}\gamma a^2)\}]\partial V/\partial f. \tag{28}$$

In the case where V is given by the ϕ^4 potential (3), these equations admit nonlinear periodic solutions (Henry *et al.* 1982). It is instructive to proceed by considering solutions for the particular velocity

$$c = \{\gamma a^2/4(M_1 M_2)^{\frac{1}{2}}\}^{\frac{1}{2}}. \tag{29}$$

Equation (27) now becomes a second-order nonlinear differential equation which can be written in the form

$$(M_1+M_2)(c^2 - c_A^2)\frac{\mathrm{d}^2 f}{\mathrm{d}s^2} + \frac{\partial V}{\partial f} = -\frac{c^2 M_2}{2\gamma}\frac{\mathrm{d}^2}{\mathrm{d}s^2}\left(\frac{\partial V}{\partial f}\right). \tag{30}$$

The LHS of this equation is identical to the KS equation for a monatomic chain (their equation 6), with the single mass replaced by $M_1 + M_2$, generalized to include

a range of potentials (Currie *et al.* 1980). To a first approximation (Büttner and Bilz 1978) the terms on the RHS renormalize coupling constants for small amplitudes. In the case where V is the ϕ^4 potential, Büttner and Bilz (1978, 1981) have derived a similar equation to describe (i) optic mode solitary waves in a diatomic chain with harmonic and quartic nearest neighbour interactions and (ii) the relative electron–ion displacement in a model ferroelectric in the adiabatic approximation.

Equation (30) can be solved using standard techniques (Ames 1968). First, we make the substitutions

$$\mathrm{d}f/\mathrm{d}s = p, \qquad \mathrm{d}^2f/\mathrm{d}s^2 = p\,\mathrm{d}p/\mathrm{d}f,$$

to arrive at

$$\frac{\mathrm{d}p}{\mathrm{d}f} = \frac{-c^2M_2\,p^2\,\partial^3V/\partial f^3 + 2\gamma\,\partial V/\partial f}{\alpha_0\,p + c^2M_2\,p\,\partial^2V/\partial f^2} = -\frac{(Pp,f)}{Q(p,f)}, \tag{31}$$

where $\alpha_0 = 2\gamma(M_1+M_2)(c^2-c_A^2)$. Now, using the integrating factor

$$\lambda(p,f) = \alpha_0 + c^2M_2\,\partial^2V/\partial f^2,$$

we can construct the exact differential

$$\lambda P\,\mathrm{d}f + \lambda Q\,\mathrm{d}p = 0. \tag{32}$$

Hence, if we define $\psi(p,f)$ such that

$$\partial\psi/\partial f = \lambda P, \qquad \partial\psi/\partial p = \lambda Q,$$

then

$$\psi(p,f) = 0. \tag{33}$$

Solving equation (33) for p, and hence s, results in

$$s = \int \frac{c^2M_2\,\partial^2V/\partial f^2 + \alpha_0}{\{C - 2\gamma c^2M_2(\partial V/\partial f)^2 - 4\gamma\alpha_0 V\}^{\frac{1}{2}}}\,\mathrm{d}f. \tag{34}$$

In general, the solutions of (34) involve complicated expressions with hyper-elliptic integrals. However, with V given by equation (3), and choosing

$$C = \frac{4\gamma(\alpha_0 - c^2M_2A)^2}{3c^2M_2B}\left(A + \frac{B(\alpha_0 - c^2M_2A)}{9c^2M_2B}\right),$$

we obtain the simple solution

$$f = f_0\sin(ks), \tag{35}$$

where $k = (2\gamma/9c^2M_2)^{\frac{1}{2}}$. The corresponding solution for g is

$$g = g_0\sin(ks) + g_1\sin(3ks). \tag{36}$$

The amplitudes of these nonlinear periodic solutions are determined explicitly by the parameters of the problem. With an appropriate change of amplitude, these

solutions also solve the original equations of motion (9) exactly! The amplitudes of these exact nonlinear phonon solutions are found to be

$$f_0 = \big((4/3B)[M_1 M_2 c^4 k^4 - \{2\gamma(M_1+M_2) - AM_2\}c^2k^2 - 2A\gamma + \gamma^2 a^2 k^2 - \tfrac{1}{16}\gamma^2 a^4 k^4]/(M_2 c^2 k^2 - 2\gamma)\big)^{\frac{1}{2}}, \tag{37a}$$

$$g_0 = \frac{2\gamma - \frac{1}{4}\gamma a^2 k^2}{2\gamma - M_2 c^2 k^2} f_0, \qquad g_1 = \frac{B}{9\gamma a^2 k^2 - 8\gamma} f_0^3, \tag{37b, c}$$

where the velocity is related to the wavevector by

$$c = (2\gamma/9k^2 M_2)^{\frac{1}{2}}. \tag{38}$$

Hence, these solutions oscillate with the characteristic frequency

$$\omega = ck = (2\gamma/9M_2)^{\frac{1}{2}}. \tag{39}$$

The nonlinear phonons of equations (35)–(38) are high energy phonons. We note that the frequency and wavelength of low amplitude nonlinear phonons with $g_1 \ll f_0 \ll 1$ is related by

$$\omega^2 \approx \frac{2\gamma(M_1+M_2) - AM_2}{2M_1 M_2}\left\{1 \pm \left(1 - \frac{4(\gamma^2 a^2 k^2 - 2A\gamma - \frac{1}{16}\gamma^2 a^4 k^4)M_1 M_2}{\{2\gamma(M_1+M_2) - AM_2\}^2}\right)^{\frac{1}{2}}\right\}. \tag{40}$$

This is found by taking $f_0 \to 0$ in equation (37a). In the long wavelength limit, the dispersion relation (40) has the two branches

$$\omega^2(-) \approx (\gamma^2 a^2 k^2 - 2A\gamma)/\{2\gamma(M_1+M_2) - AM_2\}, \tag{41}$$

$$\omega^2(+) \approx \{2\gamma(M_1+M_2) - AM_2\}/M_1 M_2 - \omega^2(-). \tag{42}$$

The lower branch $\omega^2(-)$, which is defined for $k > (2A/a^2\gamma)^{\frac{1}{2}}$, reduces to the KS dispersion relation for linearized high energy phonons (their equation 12) in the limit $M_2 \to 0$.

We note that solutions analogous to the nonlinear phonons discussed above, also solve the discrete equations of motion (6) exactly. These 'periodon' solutions are (Büttner and Bilz 1981)

$$u_n = F_0 \sin(\omega t - nqa), \tag{43a}$$

$$v_n = G_0 \sin\{\omega t - (n+\tfrac{1}{2})qa\} + G_1 \sin[3\{\omega t - (n+\tfrac{1}{2})qa\}], \tag{43b}$$

with amplitudes

$$F_0 = \big((4/3B)[M_1 M_2 \omega^4 - \{2\gamma(M_1+M_2) - AM_2\}\omega^2 - 2A\gamma + 4\gamma^2 \sin^2(\tfrac{1}{2}qa)]/(\omega^2 M_2 - 2\gamma)\big)^{\frac{1}{2}}, \tag{44a}$$

$$G_0 = \frac{2\gamma \cos(\frac{1}{2}qa)}{2\gamma - \omega^2 M_2} F_0, \qquad G_1 = -\frac{B}{8\gamma \cos(\frac{3}{2}qa)} F_0^3, \tag{44b, c}$$

and frequency

$$\omega = (2\gamma/9M_2)^{\frac{1}{2}}. \tag{45}$$

In the long wavelength limit, $qa \ll 1$, we replace the discrete index na by a continuous variable x and recover the nonlinear phonons of equations (35)–(38). Thus, the nonlinear phonons are the continuum analogue of discrete lattice periodons.

In the Appendix we show that the large amplitude kink and nonlinear periodic solutions derived above can also be found in the displacive regime of the model Hamiltonian (5), generalized to include single well potentials on the M_2 species.

4. Numerical Investigation of the Diatomic Chain

Since the kink solutions discussed in Section 3 are topologically stable finite energy excitations it is expected that they will be important [for example, contribute a tunnelling term (Krumhansl and Schrieffer 1975)] in the statistical mechanics of the diatomic chain. This leads us to an investigation of the field equations for kink configurations at velocities other than the characteristic velocity $c = c_0$. It can be shown by direct substitution that the field equations cannot support a kink solitary wave having a hyperbolic tangent profile for velocities $c \neq c_0$. To investigate the coupled field equations for more general kink configurations we have studied our equations using numerical techniques. The discrete equations of motion have also been studied numerically, using the molecular dynamics technique (Schneider and Stoll 1973, 1976; Koehler *et al.* 1975).

Introducing the dimensionless quantities

$$\xi = u/u_0, \quad \eta = v/u_0, \quad \bar{\gamma} = \gamma/A, \quad \bar{c} = a^{-1}(M_1/A)^{\frac{1}{2}}c, \quad \bar{m} = M_2/M_1 \tag{46}$$

into the field equations (9) with the ϕ^4 on-site potential, and performing some elementary manipulations, we write our equations of motion in the form

$$F_1(\xi_{ss}, \xi, \eta) = \xi_{ss} + \bar{\gamma}(1 - 4\bar{m}\bar{c}^2\bar{\gamma}^{-1})(\xi - \eta) + 2\bar{m}\bar{c}^2\bar{\gamma}^{-1}(\xi - \xi^3) = 0, \tag{47a}$$

$$F_2(\eta_{ss}, \xi, \eta) = \eta_{ss} + \bar{\gamma}(1 - 4\bar{c}^2\bar{\gamma}^{-1})(\eta - \xi) + \tfrac{1}{2}(\xi - \xi^3) = 0, \tag{47b}$$

with

$$s = (x - ct)/d; \quad d = [2\bar{m}\bar{c}^2\bar{\gamma}^{-1}\{\bar{\gamma}^2(16\bar{m}\bar{c}^2)^{-1} - \bar{c}^2\}]^{\frac{1}{2}}a. \tag{48}$$

By defining

$$\boldsymbol{Y}_{(s)} = \begin{bmatrix} \xi \\ \xi_s \\ \eta \\ \eta_s \end{bmatrix}, \qquad \boldsymbol{F}_{(s)} = \begin{bmatrix} \xi_s \\ \bar{\gamma}(1 - 4\bar{m}\bar{c}^2\bar{\gamma}^{-1})(\eta - \xi) + 2\bar{m}\bar{c}^2\bar{\gamma}^{-1}(\xi^3 - \xi) \\ \eta_s \\ \bar{\gamma}(1 - 4\bar{c}^2\bar{\gamma}^{-1})(\xi - \eta) + \tfrac{1}{2}(\xi^3 - \xi) \end{bmatrix}, \tag{49a, b}$$

the coupled equations of motion (47) can be written as a first-order system

$$\mathrm{d}\boldsymbol{Y}_{(s)}/\mathrm{d}s = \boldsymbol{F}_{(s)}. \tag{50}$$

We now introduce a first integral of motion which can be used to transform the boundary conditions for a given configuration into a relation between the initial conditions (Subbaswamy and Trullinger 1979). We construct a first integral here from an appropriate linear combination of the integrals

$$\int F_1(\xi_{ss}, \xi, \eta)\xi_s \, \mathrm{d}s, \qquad \int F_2(\eta_{ss}, \xi, \eta)\xi_s \, \mathrm{d}s,$$

$$\int F_1(\xi_{ss}, \xi, \eta)\eta_s \, \mathrm{d}s, \qquad \int F_2(\eta_{ss}, \xi, \eta)\eta_s \, \mathrm{d}s.$$

Explicitly we derive the relation

$$-2\bar{c}^2\bar{\gamma}^{-1}\xi_s^2+\xi_s\eta_s-2mc^2\bar{\gamma}^{-1}\eta_s^2+\bar{\gamma}(1-16\bar{m}\bar{c}^4\bar{\gamma}^{-2}\xi\eta)$$
$$+\{\tfrac{1}{4}(1-16\bar{m}\bar{c}^4\bar{\gamma}^{-2})+2\bar{c}^2(1-\tfrac{1}{4}\bar{\gamma}\bar{c}^{-2})\}\xi^2-\tfrac{1}{2}\bar{\gamma}(1-16\bar{m}\bar{c}^4\bar{\gamma}^{-2})\eta^2$$
$$-\tfrac{1}{8}(1-16\bar{m}\bar{c}^4\bar{\gamma}^{-2})\xi^4=C. \tag{51}$$

The integration constant C is chosen to fit the boundary conditions for a given configuration. Using the kink boundary conditions

$$\xi|_{s=\pm\infty}=\pm1,\quad \eta|_{s=\pm\infty}=\pm1,\quad \xi_s|_{s=\pm\infty}=0,\quad \eta_s|_{s=\pm\infty}=0, \tag{52}$$

we obtain

$$C=\tfrac{1}{8}+\tfrac{1}{2}\bar{\gamma}\alpha\bar{m}^{-1}-(\tfrac{1}{2}\bar{\gamma}+\tfrac{1}{8})\alpha^2\bar{m}^{-1}, \tag{53}$$

where $\alpha=4\bar{m}\bar{c}^2\bar{\gamma}^{-1}$. The boundary value problem is now reduced to an initial value problem with the initial conditions $\xi(0)$, $\eta(0)$, $\xi_s(0)$ and $\eta_s(0)$ related by equations (51) and (53). Without loss of generality we take $\xi(0)=0$, then the remaining initial conditions are related through

$$\eta_s(0)=\{\xi_s(0)/\alpha\}(1\pm\beta^{\frac{1}{2}}), \tag{54}$$

where

$$\beta=1-\alpha[\alpha\bar{m}^{-1}+\xi_s^{-2}(0)\{\bar{\gamma}(1-\alpha^2\bar{m}^{-1})\eta^2(0)+2C\}]. \tag{55}$$

We now specify $\eta^2(0)$, α and β, and derive the initial conditions $\xi_s(0)$ and $\eta_s(0)$ using equations (54) and (55).

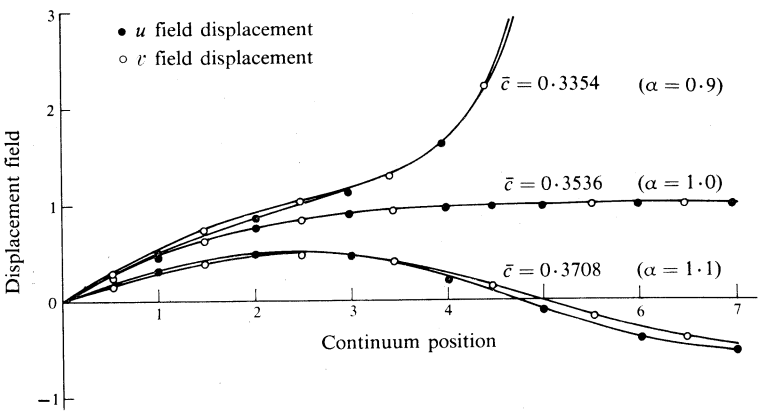

Fig. 3. Variation of u and v field displacements with continuum position for three different velocities $\bar{c}$, using $\bar{\gamma}=1$, $\bar{m}=2$, $\eta^2(0)=0$ and $\beta=0$.

Employing the above numerical scheme we have investigated the equations of motion using a fourth-order Runge–Kutta initial value routine for several sets of the parameters $\eta^2(0)$, α and β in the range $[0,2]$. In all cases, the dimensionless coupling was taken to be $\bar{\gamma}=1$ (displacive regime), and the mass ratio was taken to be $\frac{1}{2}$ or 2. We were unable to obtain solutions with domain wall like profiles except in the special case $\bar{m}=2$, $\eta^2(0)=0$, $\alpha=1$ and $\beta=0$. In this case we recovered

the kink solitary wave solution found analytically in Section 3. In Fig. 3 we show numerical solutions generated using $\bar{\gamma} = 1$, $\bar{m} = 2$, $\eta^2(0) = 0$ and $\beta = 0$. Solutions for three different velocities $\bar{c} = (\alpha\bar{\gamma}/4\bar{m})^{\frac{1}{2}}$ are shown. It can be seen that for $\alpha = 0{\cdot}9$ (or $\alpha < 1$) the solutions diverge rapidly, and for $\alpha = 1{\cdot}1$ ($\alpha > 1$) the solutions oscillate. However, in the case $\alpha = 1$, the displacement fields are equal and produce a kink profile.

Kink configurations have been found to occur in the discrete chain, for a range of velocities and mass ratios. These profiles were generated using the molecular dynamics (MD) technique. This technique directly integrates Newton's equations of motion for a given Hamiltonian and it is the most direct technique that can be used to calculate time-dependent properties of an arbitrary classical many body problem (Koehler and Lee 1976).

We write the discrete equations of motion (6) in the convenient computational form

$$\mathrm{d}^2\xi_n/\mathrm{d}\bar{t}^2 = -\xi_n^3 + (1-2\bar{\gamma})\xi_n + \bar{\gamma}(\eta_n + \eta_{n-1}), \tag{56a}$$

$$\bar{m}\,\mathrm{d}^2\eta_n/\mathrm{d}\bar{t}^2 = -2\bar{\gamma}\eta_n + \bar{\gamma}(\xi_{n+1} + \xi_n), \tag{56b}$$

where $\bar{t} = (A/M_1)^{\frac{1}{2}}t$ and the other dimensionless parameters are defined by equations (46). The MD simulation is started with the initial positions and velocities of particles in the chain chosen to represent a typical low energy configuration. The Verlet central difference algorithm

$$\Gamma_n(t+h) = 2\Gamma_n(t) - \Gamma_n(t-h) + h^2\ddot{\Gamma}_n(t), \tag{57}$$

with $\Gamma_n = \xi_n, \eta_n$, is then used to generate positions at time $t+h$ from those at time t. Velocities $\dot{\Gamma}_n = \dot{\xi}_n, \dot{\eta}_n$ at time t are calculated from

$$\dot{\Gamma}_n(t) = \{\Gamma_n(t+h) - \Gamma_n(t-h)\}/2h. \tag{58}$$

The zero of time for the system is taken after several thousand steps in order to eliminate any initial bias. The dimensionless temperature of the chain $\bar{T} = k_B TBA^{-2}$ is calculated from

$$\bar{T} = \tfrac{1}{2}\langle\bar{\dot{\xi}}^2 + \bar{m}\bar{\dot{\eta}}^2\rangle, \tag{59}$$

where $\bar{\dot{\xi}}^2$ and $\bar{\dot{\eta}}^2$ are the mean square velocities of M_1 and M_2 type atoms respectively, and the angle brackets denote the time average over a run.

We performed an MD simulation of our model with a step size of $h = 0{\cdot}2$ for a system of 2000 particles subject to periodic boundary conditions. The MD run was initiated with particles randomly displaced a small distance from the ground state configuration $\xi = \eta = -1$. We have made plots of the displacements of the first 1000 particles in the chain after 5000 integration steps for a range of temperatures ($\bar{T} \approx 0{\cdot}06, 0{\cdot}10, 0{\cdot}14$) in the displacive ($\bar{\gamma} = 1$) regime. These are shown in Figs 4*a* and 4*b* for the two mass ratios $\bar{m} = 0{\cdot}5$ and $2{\cdot}0$ respectively. Profiles with domain wall (kink) like structure can be easily identified at $\bar{T} \approx 0{\cdot}10$ for both mass ratios. Furthermore, the increase in kink density with temperature is clearly observable.

We are presently extending our MD calculations over a wide range of parameters. A calculation of the structure factor from our MD data is also in progress.

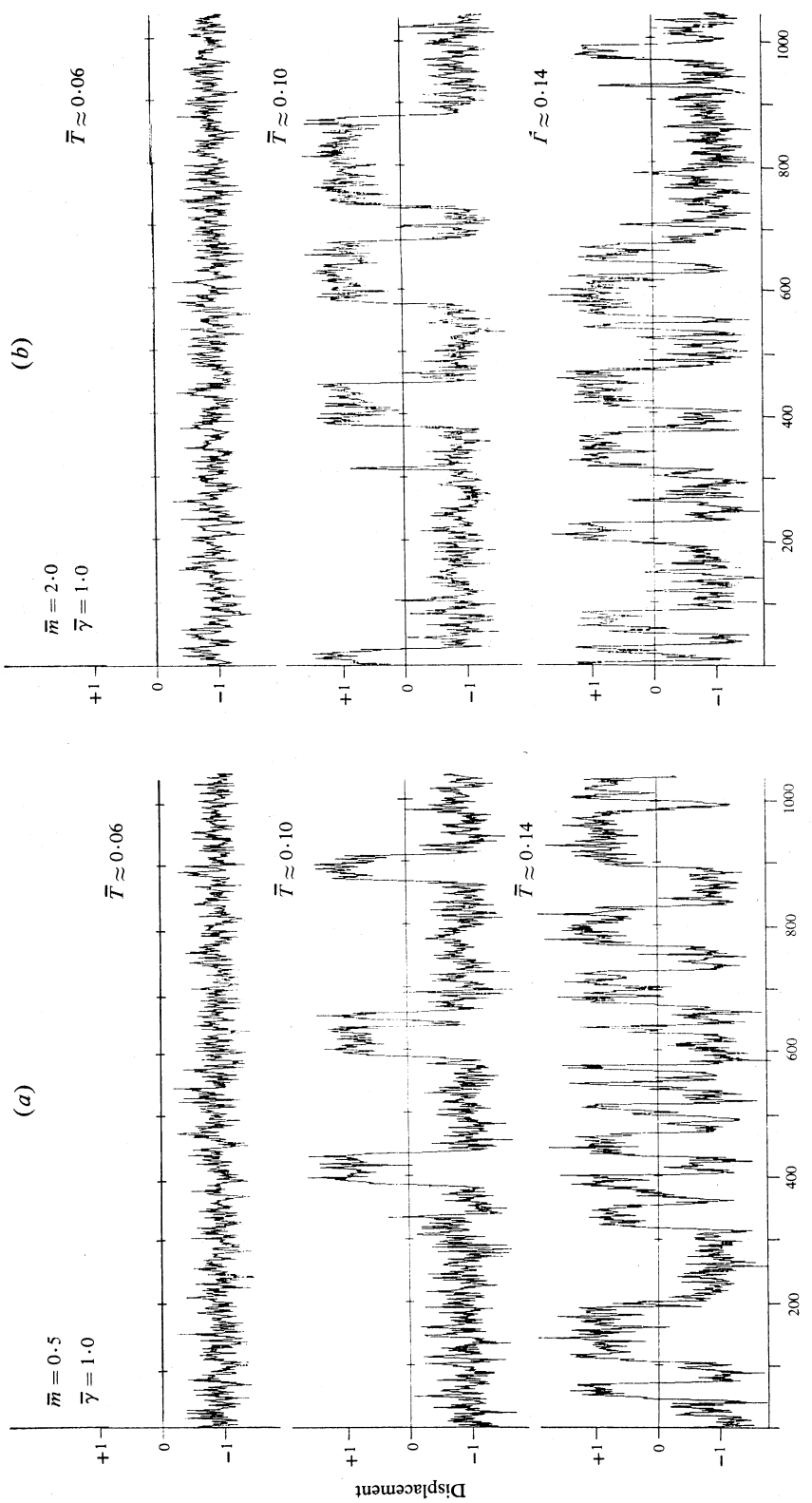

Fig. 4. Displacements at 1000 lattice sites for a range of temperatures $\bar{T}$ in the displacive ($\bar{\gamma} = 1$) regime. The mass ratios M_2/M_1 are (*a*) 0·5 and (*b*) 2·0.

5. Statistical Mechanics Considerations

The classical partition function for the nonlinear diatomic chain can be written as the functional integral

$$Z(\dot{u},\dot{v},u,v) = \int \delta(\dot{u})\,\delta(\dot{v})\,\delta(u)\,\delta(v)\exp\left(-\beta\int\frac{\mathrm{d}x}{a}\tilde{H}\right), \tag{60}$$

with the Hamiltonian density defined by equation (8). The dominant contribution to the partition function comes from the steepest descent trajectories which are described by the Euler–Lagrange equations of motion (9). Trajectories which are close to the dominant ones provide linear stability information (Scott *et al.* 1973) and are also important for thermal corrections (Bishop 1978). Thus, it is expected that the topologically stable finite energy solutions of the coupled field equations will participate actively in the statistical mechanics of the nonlinear diatomic chain.

The excitation energy corresponding to a solution of the coupled field equations is found using equation (18), together with the boundary conditions appropriate to the solution. We thus derive the kink excitation energy

$$E_{\mathrm{K}} = 2a\gamma u_0^2/3\xi_{\mathrm{K}}\,. \tag{61}$$

The pulse energy is found to be infinite for all values of the parameters. The excitation energy of the nonlinear phonon (NP) solutions on a chain of length L is

$$E_{\mathrm{NP}} = a_0 L + a_1\cos\{2(2\gamma/9M_2)^{\frac{1}{2}}t\}\sin(kL) + a_2\cos\{4(2\gamma/9M_2)^{\frac{1}{2}}t\}\sin(2kL), \tag{62}$$

where the constants a_0, a_1 and a_2 depend on the parameters of the model. In particular, finite energy nonlinear phonons are possible for parameters satisfying $a_0 = 0$.

The ground state of our nonlinear diatomic chain is similar to the ground state of the corresponding monatomic chain. In both cases, the manifold of internal states (Toulouse and Kléman 1976) is simply the two points ± 1. Clearly both chains are also of the same dimensionality and hence, topological considerations follow directly. In particular, the kink solution, which is a minimum energy path between the two states, is topologically stable whereas the pulse solution, which never approaches either state, is non-topological.

The above preliminary considerations involving energetics and stability suggest that a configurational phenomenology for the statistical mechanics of the diatomic chain should involve kinks, linear phonons, nonlinear phonons and interactions between these modes. For example, mode coupling is expected between nonlinear phonons and linear phonons with the same wavelength and frequency. Using the low energy linear phonon dispersion relation (10) in equation (37a), we obtain mode coupled nonlinear phonons of amplitude $f_0 = 2u_0$. In general, interactions between linear phonons and nonlinear modes produce a translation mode. We derive the translation mode by considering a small perturbation on the solutions $u_{\mathrm{s}}(s)$ and $v_{\mathrm{s}}(s)$ of our equations of motion. We thus make the substitutions

$$u(x,t) = u_{\mathrm{s}}(s) + \phi(s)\exp(-\mathrm{i}\,\omega t), \tag{63a}$$

$$v(x,t) = v_{\mathrm{s}}(s) + \psi(s)\exp(-\mathrm{i}\,\omega t), \tag{63b}$$

in equations (20). Retaining terms only linear in ϕ and ψ we arrive at the linear stability equations

$$M_1 c^2 \frac{d^2\phi}{ds^2} + 2\gamma(\phi - \psi) - \tfrac{1}{4}\gamma a^2 \frac{d^2\psi}{ds^2} - A\phi + 3B u_s^2(s)\phi = \omega^2 M_1 \phi - i(2\omega c M_1)\frac{d\phi}{ds}, \quad (64a)$$

$$M_2 c^2 \frac{d^2\psi}{ds^2} + 2\gamma(\psi - \phi) - \tfrac{1}{4}\gamma a^2 \frac{d^2\phi}{ds^2} = \omega^2 M_2 \psi - i(2\omega c M_2)\frac{d\psi}{ds}. \quad (64b)$$

It is easy to show that the zero frequency eigenfunctions of these equations are

$$\phi = s_0\, du_s(s)/ds, \qquad \psi = s_0\, dv_s(s)/ds, \quad (65a, b)$$

where s_0 is a small amplitude. Substituting $f(s) = u_s(s) = v_s(s)$ into (20), and differentiating with respect to s, leads to

$$M_1 c^2 \frac{d^2}{ds^2}\left(\frac{du_s(s)}{ds}\right) + 2\gamma\left(\frac{du_s(s)}{ds} - \frac{dv_s(s)}{ds}\right) - \tfrac{1}{4}\gamma a^2 \frac{d^2}{ds^2}\left(\frac{dv_s(s)}{ds}\right) - A\frac{du_s(s)}{ds} + 3B u_s^2(s)\frac{du_s(s)}{ds} = 0, \quad (66a)$$

$$M_2 c^2 \frac{d^2}{ds^2}\left(\frac{dv_s(s)}{ds}\right) + 2\gamma\left(\frac{dv_s(s)}{ds} - \frac{du_s(s)}{ds}\right) - \tfrac{1}{4}\gamma a^2 \frac{d^2}{ds^2}\left(\frac{du_s(s)}{ds}\right) = 0. \quad (66b)$$

Thus, comparing equations (64) and (66) shows that equations (65) are solutions of (64) with $\omega^2 = 0$.

The physical interpretation of these perturbations comes from substituting equations (65) into (63) with $\omega = 0$. To first order in s_0 this yields

$$u(x, t) \approx u_s(s + s_0), \qquad v(x, t) \approx v_s(s + s_0). \quad (67a, b)$$

Thus, these solutions are translation modes and are similar to the zero frequency translation modes reported in nonlinear monatomic chains (Scott *et al.* 1973; Bishop *et al.* 1980; Currie *et al.* 1980).

6. Summary

We have examined the field equations for the continuum description of a diatomic chain, including a nonlinear potential on one species. This model may be relevant to solids which undergo displacive structural phase transitions. We have identified three types of excitation in this chain. These are low amplitude linearized phonons, large amplitude nonlinear phonons, and large amplitude equal displacement field solitary waves.

The nonlinear periodic solution is the continuum analogue of discrete lattice periodons. This excitation is a higher energy solution than the linearized phonons.

The equal displacement field solitary waves take the form of a topologically stable kink or unstable pulse, depending on the mass ratio. The speed of propagation of these solitary waves is fixed by the parameters of the problem. Further, a numerical

investigation of the field equations has failed to reveal kink-type excitations for other velocities or mass ratios. This is in contrast to discrete lattice domain walls, generated using the molecular dynamics technique, which occur for both mass ratios and a range of velocities.

The finite energy solutions, including linearized and nonlinear phonons and kinks, of our coupled field equations, together with mode interactions (e.g. translation mode), should all be included in a basis for calculating thermodynamic functions in our chain.

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Appendix. Diatomic Chain with Double Well Potentials on One Species and Single Well Potentials on the Other Species

Here we present kink solutions and nonlinear periodic solutions in the displacive regime of the model Hamiltonian

$$H = \sum_i \{\tfrac{1}{2}M_1 \dot{u}_i^2 + \tfrac{1}{2}M_2 \dot{v}_i^2 + \tfrac{1}{2}\gamma(u_i - v_i - 1)^2 + \tfrac{1}{2}\gamma(u_i - v_i)^2 + V(u_i) + U(v_i)\}. \tag{A1}$$

This is an extension of the model Hamiltonian (8) to include the single well potentials

$$U(v) = \alpha \tfrac{1}{2} A v^2 \tag{A2}$$

on the M_2 species. Depending on the relative strengths of the coupling γ and the potential α, two distinct ground state configurations are possible. In the order–disorder regime of this model, dealt with by Subbaswamy and Mills (1978), the ground state is $u = \pm u_0$ and $v = 0$. In the displacive regime where $\gamma/A > \frac{1}{2}\alpha$ the ground state is as before, $u = v = \pm u_0$.

Solitary waves are now obtained for the characteristic velocity

$$c_\beta = (\gamma a^2 \beta / 4M_2)^{\frac{1}{2}}, \tag{A3}$$

where $\beta = (2\gamma + \alpha A)/2\gamma$. Explicitly we obtain for $M_1 \beta^2 < M_2$

$$v(x,t) = \beta^{-1} u(x,t) = \pm u_\beta \tanh(s/\xi_\beta), \tag{A4}$$

where

$$u_\beta = \left(\frac{A - 2\gamma + 2\gamma/\beta}{\beta}\right)^{\frac{1}{2}}, \qquad \xi_\beta = \left(\frac{2c^2(M_2/\beta^2 - M_1)}{A - 2\gamma + 2\gamma/\beta}\right)^{\frac{1}{2}}.$$

At other velocities $c \neq c_\beta$ the following nonlinear periodic solutions may be found:

$$u = \tilde{f}_0 \sin\{k(x - ct)\}, \tag{A5a}$$

$$v = \tilde{g}_0 \sin\{k(x - ct)\} + \tilde{g}_1 \sin\{3k(x - ct)\}, \tag{A5b}$$

where

$$\tilde{f}_0 = \big((4/3B)[M_1 M_2 \omega^4 - \{2\gamma(M_1 + M_2) - AM_2 + \alpha A M_1\}\omega^2 - 2\gamma(1 - \alpha)A - \alpha A^2 + \gamma^2 a^2 k^2 - \tfrac{1}{16}\gamma^2 a^4 k^4]/(M_2 \omega^2 - 2\gamma + \alpha A)\big)^{\frac{1}{2}}, \tag{A6a}$$

$$\tilde{g}_0 = \frac{2\gamma - \frac{1}{4}\gamma a^2 k^2}{2\gamma + \alpha A - \omega^2 M_2} f_0, \qquad \tilde{g}_1 = \frac{B}{9\gamma a^2 k^2 - 8\gamma} f_0^3, \tag{A6b,c}$$

with frequency

$$\omega = \{(2\gamma + \alpha A)/9M_2\}^{\frac{1}{2}}. \tag{A7}$$

The velocity of these solutions is

$$c = \{(2\gamma + \alpha A)/9M_2 k\}^{\frac{1}{2}}. \tag{A8}$$

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