Solitary waves in a diatomic lattice: analytic approximations for a wide range of speeds by quasi-continuum methods

Jonathan A.D. Wattis

Division of Theoretical Mechanics, School of Mathematical Sciences, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

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Abstract

We extend the quasi-continuum method of approximation to find waves of general speed in a diatomic lattice. Our results include as a special case the one speed which previous methods have found; we find the shape of nonlinear waves of arbitrary velocity up to some maximum speed. © 2001 Published by Elsevier Science B.V.

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1. Introduction

The use of quasi-continuum methods in determining the form of solitary waves in nonlinear lattice problems was established by Collins [2] and Rosenau [7]. The properties of such partial differential equations and their solutions was investigated even earlier by Benjamin et al. [1], who noted that more accurate dispersion relations could be achieved by regularising long wave equations. However, due to the complexity of resulting partial differential equations, the quasi-continuum method has largely been restricted to monoatomic lattices in one dimension. Notable exceptions to this include Pnevmatikos et al. [5] and Pnevmatikos et al. [6], who study diatomic lattices in which atoms interact only with their nearest neighbours via nonlinear springs, and Peyrard et al. [4] in which the nonlinear nearest-neighbour interactions replaced by a combination of on-site potentials and an interaction term. Previous approaches to modelling diatomic systems by Peyrard et al. [3,4] have found the shape of the nonlinear wave only for one particular wave speed, referred to as \( v_0 \). In [4] Peyrard et al. also numerically show that faster waves (with speed \( v > v_0 \)) radiate energy slowing to \( v_0 \); they also present results which suggest the existence of slower waves, with velocities as low as zero.

In this Letter we find formulae for the shape of waves encompassing both the \( v < v_0 \) and \( v > v_0 \) ranges of wave speed. Following the notation of Cretegny and Peyrard [3] we write the Hamiltonian of the system as

\[ H = \sum_{n=1}^{N} \left( \frac{1}{2} p_n^2 + V(x_n) - \frac{1}{2} \sum_{m \neq n}^{N} \frac{1}{1 + \alpha^2 |x_n - x_m|^2} \right) \]

where \( p_n \) and \( x_n \) are the momentum and displacement of the \( n \)-th atom, respectively, \( V(x_n) \) is the on-site potential, and \( \alpha \) is the coupling constant. The Hamiltonian is then approximated by replacing the discrete sum with a continuum integral:

\[ H_{\text{cont}} = \int \left( \frac{1}{2} \rho \dot{u}^2 + V(u) - \frac{1}{2} \int \frac{1}{1 + \alpha^2 |x - y|^2} \rho \dot{u} \dot{y} \right) \, dx \]

where \( u(x) \) is the continuum approximation to the lattice displacement and \( \rho \) is the mass density.

\[ E(u) = \int \left( \frac{1}{2} \rho \dot{u}^2 + V(u) - \frac{1}{2} \int \frac{1}{1 + \alpha^2 |x - y|^2} \rho \dot{u} \dot{y} \right) \, dx \]


E-mail address: jonathan.wattis@nottingham.ac.uk (J.A.D. Wattis).

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\[ H = H_P + H_O + H_{\text{int}}, \text{ where} \]
\[
H_P = \sum_n \frac{1}{2} m \dddot{u}_n^2 + \varepsilon_0 \left( 1 - \frac{u_n^2}{u_0^2} \right)^2 + \frac{1}{2} k_1 (u_{n+1} - u_n)^2, \quad (1.1)
\]
\[
H_O = \sum_n \frac{1}{2} M \dddot{\varrho}_n^2 + \frac{1}{2} K_0 \varrho_n^2 + \frac{1}{2} K_1 (\varrho_{n+1} - \varrho_n)^2, \quad (1.2)
\]
\[
H_{\text{int}} = \sum_n \chi \varrho_n (u_n^2 - u_0^2), \quad (1.3)
\]

and the subscript \( P \) refers to the light, proton sublattice, with displacements \( u_n(t) \) and masses \( m \); the \( O \) subscript refers to the heavy, oxygen sublattice, with displacements \( \varrho_n(t) \) and masses \( M \). Each site of the lattice interacts with its second neighbour (which is its nearest neighbour of the same sublattice) through a linear spring of constant \( k_1 \) for the light sublattice and constant \( K_1 \) for the heavy sublattice. In addition, the lighter atoms experience an onsite double-well potential, and the heavier atoms, a single-well. The sublattices interact through one term, namely the interaction energy, \( H_{\text{int}} \).

The equations of motion for the system are thus
\[
m \dddot{u}_n = k_1 (u_{n+1} - 2u_n + u_{n-1}) + \frac{4\varepsilon_0}{u_0^2} \left( 1 - \frac{u_n^2}{u_0^2} \right) u_n - 2\chi \varrho_n u_n, \quad (1.4)
\]
\[
M \dddot{\varrho}_n = K_1 (\varrho_{n+1} - 2\varrho_n + \varrho_{n-1}) - K_0 \varrho_n - \chi (u_n^2 - u_0^2). \quad (1.5)
\]

The parameters \( K_0 \) and \( K_1 \) are wrongly swapped in [3], along with an error in the definition of \( \mu \) in Eq. (10) which is corrected in (1.13) below. The classic travelling wave solution is found by taking the continuum limit of these equations, to yield the partial differential equations
\[
m \dddot{u} = k_1 \dddot{u} \dddot{z} + \frac{4\varepsilon_0}{u_0^2} \left( 1 - \frac{u^2}{u_0^2} \right) u - 2\chi \varrho \dddot{u}, \quad (1.6)
\]
\[
M \dddot{\varrho} = K_1 \dddot{\varrho} \dddot{z} - K_0 \dddot{\varrho} - \chi (u^2 - u_0^2), \quad (1.7)
\]

for \( u(x, t) = u(an, t) \) and \( \varrho(x, t) = \varrho(an, t) \) which replace \( u_n(t) \) and \( \varrho_n(t) \), respectively; here, \( a \) is the lattice spacing. We seek a solution which travels at speed \( v \), thus \( u(z) = u(x - vt) \) and \( \varrho(z) = \varrho(x - vt) \) satisfy
\[
v^2 \dddot{\varrho} = K_1 v^2 \dddot{\varrho} - K_0 \dddot{\varrho} - \chi (u^2 - u_0^2), \quad (1.8)
\]
\[
v^2 \dddot{u} = k_1 v^2 \dddot{u} + \frac{4\varepsilon_0}{u_0^2} \left( 1 - \frac{u^2}{u_0^2} \right) u - 2\chi \varrho \dddot{u}, \quad (1.9)
\]

where prime denotes differentiation with respect to \( z \). In previous studies [3,4] the assumption on the wave speed of \( v = v_0 = a \sqrt{K_1/M} \) is made yielding a simple form for \( \varrho(z) \) from (1.8),
\[
\varrho = \frac{-\chi}{K_0} (u^2 - u_0^2), \quad (1.10)
\]

which can be substituted into (1.9), to yield a tractable equation. We also substitute
\[
o_0^2 = \frac{4\varepsilon_0}{mu_0^2}, \quad o_1^2 = \frac{k_1}{m}, \quad \Omega_0^2 = \frac{K_0}{M}, \quad \Omega_1^2 = \frac{K_1}{M}, \quad (1.11)
\]

and find
\[
u(x, t) = \pm u_0 \tanh (\mu (x - v_0 t - x_0)), \quad \varrho(x, t) = \varrho_0 \sech^2 (\mu (x - v_0 t - x_0)), \quad (1.12)
\]
where
\[
\varphi_0 = \frac{x u_0^4}{K_0}, \quad \mu^2 = \frac{2 \varepsilon_0}{a^2 k_1 u_0^4} \left( 1 - \frac{x^2 u_0^4}{2 \varepsilon_0 K_0} \right) \frac{1}{1 - v_0^2/c_0^2}, \quad c_0 = a \sqrt{\frac{k_1}{m}}
\] (1.13)

Next we consider the stability of the equilibrium solution \( \varphi = 0, u = \pm u_0 \) of (1.4)–(1.5) to perturbations of the form of small amplitude linear waves of temporal frequency \( \omega \) and wavenumber \( \alpha \); thus we find the dispersion relation
\[
0 = \omega^4 - \omega^2 \left( 4 \Omega_1^2 \sin^2 \left( \frac{1}{2} \alpha s \right) + \Omega_0^2 + 4 \alpha_1^2 \sin^2 \left( \frac{1}{2} \alpha s \right) + 2 \alpha_0^2 \right)
+ \left( 4 \Omega_1^2 \sin^2 \left( \frac{1}{2} \alpha s \right) + \Omega_0^2 \right) \left( 4 \alpha_1^2 \sin^2 \left( \frac{1}{2} \alpha s \right) + 2 \alpha_0^2 \right) - \frac{4 \chi^2 u_0^2}{mM}.
\] (1.14)

This is of the form \( \omega^4 - B \omega^2 + C = 0 \), so has solutions \( \omega^2 = (1/2)(B \pm \sqrt{B^2 - 4C}) \). In order for the frequencies \( \omega \) to be real, three conditions need to be satisfied: \( B > 0, C > 0 \) and \( B^2 > 4C \). Clearly the first is satisfied, and the last is, since defining \( b_1 = 4 \Omega_1^2 \sin^2((1/2)\alpha s) + \Omega_0^2, b_2 = 4 \alpha_1^2 \sin^2((1/2)\alpha s) + 2 \alpha_0^2 \) and \( L = 4 \chi^2 u_0^2/mM \) leads to \( B = b_1 + b_2 \) and \( C = b_1 b_2 - L \) with \( L > 0 \), so that \( B^2 - 4C = (b_1 - b_2)^2 + 4L > 0 \). Thus for the stability of the discrete system of equations, the only remaining constraint on the parameters is \( C > 0 \), which reduces to
\[
\frac{4 \chi^2 u_0^2}{mM} > 2 \Omega_0^2 \alpha_0^2.
\] (1.15)

For the continuum approximation (1.6)–(1.7), we have the dispersion relation
\[
0 = \omega^4 - \omega^2 \left( a^2 \alpha_0^2 s^2 + 2 \alpha_0^2 + \Omega_0^2 + \Omega_1^2 a^2 s^2 \right)
+ \left( 2 \alpha_0^2 \Omega_0^2 - \frac{4 \chi^2 u_0^2}{mM} \right) + \Omega_0^2 \alpha_1^2 a^2 s^2 + 2 \Omega_1^2 \alpha_0^2 a^2 s^2 + \Omega_1^2 \alpha_1^2 a^4 s^4.
\] (1.16)

For small \( s \) this gives \( \omega_{ctm}^2(s)^2 = \omega(s)^2 + \mathcal{O}(s^4) \). In the limit \( s \rightarrow +\infty \), this yields \( \omega_{ctm} \sim \omega_1 a \) or \( \omega_{ctm} \sim \Omega_1 a s \). Thus the condition on the stability of the continuum limit equations (1.6)–(1.7) is also (1.15). Whilst the partial differential equations are well-posed, the high temporal frequencies of large wavenumber modes mean the approximation is not good.

2. Solution for general speed

We seek the form of the solitary wave solution for arbitrary speed, \( v \neq v_0 \). We follow the above analysis, replacing the discrete-space equations of motion (1.4)–(1.5) by the partial differential equations (1.6)–(1.7) and seeking a travelling wave solution of the system, for some speed \( v \), leading to the system of ordinary differential equations (1.8)–(1.9). Since we are considering \( v \neq v_0 \), the simple elimination (1.10) is not available. Rather, we approximate invert (1.8) to find
\[
\varphi = \frac{x}{K_0} \left[ 1 + \left( \frac{M v^2 - K_1 a^2}{K_0} \right) \frac{\partial}{\partial z} \right]^{-1} (u^2 - u_0^2) \sim \frac{x}{K_0} (u^2 - u_0^2) + \frac{2x}{K_0} \left( \frac{M v^2 - K_1 a^2}{K_0} \right) uu'.
\] (2.1)

This allows the elimination of \( \varphi \) from (1.9), yielding
\[
0 = (k_1 a^2 - m v^2) u'' + \frac{4 \varepsilon_0}{u_0^2} (1 - \frac{u^2}{u_0^2}) u + \frac{2 \chi}{K_0} (u^2 - u_0^2) u - \frac{4 \chi^2}{K_0} \left( \frac{M v^2 - K_1 a^2}{K_0} \right) uu'.
\] (2.2)
Thus we find the first integral
\[
\left( \frac{\varepsilon_0}{u_0} - \frac{\chi}{2K_0} \right) (u_0^2 - u^2)^2 = \left( \frac{1}{2} (k_1 a^2 - m v^2) \right)^2 \left( \frac{2\chi^2}{K_0} (K_1 a^2 - M v^2) u^2 \right),
\]
(2.3)
where the constant of integration has been determined by requiring \( u' = 0 \) when \( u = \pm u_0 \). In the case \( v = v_0 = a \sqrt{K_1/M} \), this equation simplifies, and solution (1.12) is recovered. Clearly both sides of (2.3) must have the same sign. For the parameters of interest to Cretegny and Peyrard [3] which are listed in the caption to Fig. 1, both sides are positive, that is, \( \varepsilon_0/u_0^4 > \chi/2K_0 \), and \( k_1 a^2 > m v^2 \). Allowing \( v \) to vary from \( v_0 \), we must maintain the positivity of the right-hand side of (2.3), this implies an extra condition on the wave speed \( v \), namely
\[
v^2 < v_{\text{max}}^2 := \frac{K_1 a^2 + 4\chi^2 u_0^4 K_1 a^2}{K_0^2 m + 4\chi^2 u_0^4 M};
\]
(2.4)
note that there is no minimum speed for such waves. Eq. (2.3) can be further integrated to yield the implicit solution
\[
2u_0 \sqrt{\frac{\varepsilon_0}{u_0^4} - \frac{\chi}{2K_0}} = 2u_0 \sqrt{B} \log(u \sqrt{B} + \sqrt{A + Bu^2})
\]
\[+ \sqrt{A + Bu_0^2} \log \left( \frac{(u - u_0)}{(u + u_0)} \frac{(A - Bu_0 u + \sqrt{A + Bu_0^2} \sqrt{A + Bu^2})}{(A + Bu_0 u + \sqrt{A + Bu_0^2} \sqrt{A + Bu^2})} \right),
\]
(2.5)
where
\[
A = \frac{1}{2} (k_1 a^2 - m v^2), \quad B = \frac{2\chi^2}{K_0} (K_1 a^2 - M v^2).
\]
(2.6)

In Fig. 1 we show the form of the solution for a range of velocities from the stationary (\( v = 0 \)) up to the maximum speed (\( v = v_{\text{max}} \)), showing that the kink waves in the \( u \)-sublattice steepen slightly at larger speeds and the corresponding pulses in the larger sublattice have an amplitude which increases with speed whilst maintaining a similar width; faster pulses also have local minima either side of the main peak. The figure has been constructed...
by plotting $\varrho$ and $z$ as functions of $u$, using (2.5) and (2.1) together with the identities $du/dz = 1/z'(u)$ and $d^2u/dz^2 = -z''(u)/z'(u)^3$. The numerical results of Peyrard et al. [4] suggest that waves which travel at speeds between $v = 0$ and $v = v_0$ exist and are stable in the lattice, however, waves with a speed greater than $v_0$ were not observed. Unfortunately, it is not possible to perform detailed stability analysis of the waves using quasi-continuum or other theoretic methods; however, it may be postulated from the numerical results of [4] that fast waves are unstable while slow waves are stable. Due to the implicit nature of the solution (2.5), it is not trivial to use the expression as initial data for numerical simulations. The above theory shows that for speeds above $v_0$, the wave in the heavy sublattice become significantly more localised, and so more susceptible to the Peierls–Nabarro potential of the discrete system. Using asymptotics it is possible to find the speed at which the pulse ceases to be single-signed; that is, the critical speed above which either side of its positive body the pulse has negative local minima and a negative tail. In the large $z$ limit, the displacement of the small atoms is determined by $u(z) \sim u_0 - u_1 e^{-z} + \cdots$. Substituting this expansion into (2.3), we find the form by which $\lambda$ depends on $v$ is

$$\lambda^2(v) = \left( \frac{4\epsilon_0}{u_0^2} - \frac{2\chi^2 u_0^2}{2K_0} \right) \left[ \frac{1}{2} (k_1 a^2 - m v^2) + \frac{2\chi^2}{K_0^2} (K_1 a^2 - M v^2) u_0^2 \right]. \quad (2.7)$$

Following (2.1), the displacements of the larger atoms is given by $\varrho \sim \varrho_1 e^{-z} + \cdots$, where

$$\varrho_1 = \frac{2au_0 \chi}{K_0} \left( 1 + \frac{\lambda^2 (K_1 a^2 - M v^2)}{K_0} \right). \quad (2.8)$$

Thus $\varrho_1$ changes sign at the speed $v_1$ where $\lambda^2(v_1) = K_0/(M v^2 - K_1 a^2)$, which enables $v_1$ to be determined from (2.7); for the parameter values used in Fig. 1, we find $v_1 = 0.57$.

3. Higher-order quasi-continuum approximations

Other partial differential equations which approximate the equations of motion (1.4)–(1.5) but which are more accurate than (1.6)–(1.7) can be constructed by forming higher-order approximations to the discrete difference operator. We follow the method of using Padé approximates used in [10] on the monoatomic discrete Klein–Gordon system, and rewrite the discrete system of Eqs. (1.4)–(1.5) in the continuous variables $u(x,t)$ and $\varrho(x,t)$ to find

$$M \varrho_{tt} = K_1 \left( a^2 \varrho_x^2 + \frac{1}{12} a^4 \varrho_x^4 + \frac{1}{360} a^6 \varrho_x^6 + \cdots \right) \varrho - K_0 \varrho - \chi (u^2 - u_0^2), \quad (3.1)$$

$$mu_{tt} = k_1 \left( a^2 \varrho_x^2 + \frac{1}{12} a^4 \varrho_x^4 + \frac{1}{360} a^6 \varrho_x^6 + \cdots \right) u + \frac{4\epsilon_0}{u_0^2} \left( 1 - \frac{u^2}{u_0^2} \right) u - 2\chi \varrho u. \quad (3.2)$$

The most straightforward higher-order continuum approximation is obtained by truncating the series after the fourth-order derivative terms to gain

$$M \varrho_{tt} = K_1 a^2 \varrho_{xx} + \frac{1}{12} K_1 a^4 \varrho_{xxxx} - K_0 \varrho - \chi (u^2 - u_0^2), \quad (3.3)$$

$$mu_{tt} = k_1 a^2 u_{xx} + \frac{1}{12} k_1 a^4 u_{xxxx} + \frac{4\epsilon_0}{u_0^2} \left( 1 - \frac{u^2}{u_0^2} \right) u - 2\chi \varrho u. \quad (3.4)$$

This equation is ill-posed, since its dispersion relation is

$$\frac{4\chi^2 u_0^2}{mM} = \left( \omega^2 - \Omega_0^2 - \Omega_1^2 a^2 s^2 + \frac{1}{12} a^4 s^4 \right) \left( \omega^2 - 2\omega_0^2 - \omega_1^2 a^2 s^2 + \frac{1}{12} \omega_1^2 a^4 s^4 \right). \quad (3.5)$$
In the limit $s \to 0$ this agrees with (1.14), the differences in $\omega^2$ being $O(s^6)$; however, as $s \to \infty$, $\omega^2 \sim -(1/12) \Omega_1^2 a^4 s^4$ or $\omega^2 \sim (1/12) \omega_1^2 a^4 s^4$, thus high wavenumber disturbances to the uniform equilibrium solution $\varrho = 0$, $u = \pm u_0$ are unstable.

However, an equally accurate approximation is obtained by forming a $(2, 2)$ Padé approximation to the discrete difference terms, replacing the approximation $a^2 \partial^2 z + (1/12) a^4 \partial^4 z$ by $(1 - (1/12) a^2 s^2) a^2 \partial^2 z$ we find

\begin{align}
M\varrho_{tt} &= K_1 a^2 \varrho_{xx} - K_0 \varrho - \chi (u^2 - u_0^2) + \frac{1}{6} a^2 \chi (uu_x)_x + \frac{1}{12} a^2 K_0 \varrho_{xx} + \frac{1}{12} a^2 M\varrho_{xx}, \tag{3.6} \\
u_{tt} &= k_1 a^2 u_{xx} + \frac{4 \epsilon_0}{u_0} (1 - \frac{u^2}{u_0^2}) u - 2 \chi \varrho u + \frac{1}{6} a^2 \chi (\varrho u)_x + \frac{a^2 \epsilon_0}{3 u_0^2} (u_{xx} - \frac{3 (u^2 u_x)_x}{u_0^2}) \\
+ \frac{1}{12} a^2 u_{xx}. \tag{3.7}
\end{align}

This system has the dispersion relation

\begin{align}
\frac{4 \chi^2 u_0^2}{m M} &= \begin{pmatrix} \omega^2 - \Omega_0^2 - \Omega_1^2 a^2 s^2 \\ 1 + (1/12) a^2 s^2 \end{pmatrix} \begin{pmatrix} \omega^2 - 2 \omega_0^2 - \frac{a^2 s^2}{1 + (1/12) \omega_1^2 a^2 s^2} \\ \omega_1^2 a^2 s^2 \end{pmatrix}, \tag{3.8}
\end{align}

which agrees with (1.14) in the limit $s \to 0$ (again the differences in $\omega^2$ are $O(s^6)$); in the limit $s \to \infty$, (3.8) implies $\omega^2 \sim 12 \Omega_1^2$ or $\omega^2 \sim 12 \omega_1^2$. While these results do not exactly agree with (1.14), they give real frequencies for both the acoustic and optical branches of the dispersion relation all wavenumbers ($s$), including the limit of large wavenumber. This is a significant improvement over (1.6)–(1.7) in that all modes of approximation (3.6)–(3.7) lie in a frequency band of finite width. Eqs. (3.6)–(3.7) thus form a stable fourth-order accurate approximation to system (1.4)–(1.5). The dispersion relations for the discrete system and all the quasi-continuum approximations are illustrated in Fig. 2.

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Fig. 2. Graphs of $\omega^2(s)$ against $s$ for the acoustic (left) and optical (right) modes, for the same parameter values as listed in Fig. 1. On both graphs the curves are, in ascending order, the ill-posed fourth-order continuum approximation (3.5), the exact dispersion relation (1.14), the well-posed fourth-order Padé approximation (3.8), and the standard second-order continuum approximation (1.16).
4. Conclusions

The results displayed in Fig. 1 show that the shape of the kink in the sublattice of small atoms is relatively independent of the speed of propagation of the wave. However, the shape of the pulse in the sublattice of larger atoms changes considerably over wave speeds from \( v = 0 \) to \( v = v_{\text{max}} \). Below a certain speed the pulse is positive in all space, whilst above this speed, the body of the pulse has a positive centre and negative edges with negative tails which decay to zero monotonically. We have determined the speed at which the pulse gains its more complicated structure by an asymptotic analysis of the tail of the wave.

In Section 3 we outlined how to construct partial differential equations which approximate the lattice equations more accurately than the standard second-order approximation. This requires the use of Padé methods to avoid the problems of ill-posedness. Fourth-order derivative terms can be included in the calculations of Section 2, generating a more accurate approximation to the shape of the solitary wave. The fourth derivative terms in (3.3)–(3.4), and the last three terms in each of (3.6)–(3.7) can be viewed as perturbations to the leading-order system (1.6)–(1.7). Thus, by substituting \( u(x, t) = u^{(0)} + u^{(1)}, \varrho(x, t) = \varrho^{(0)} + \varrho^{(1)} \) with \( u^{(0)} \) being the solution (2.5) and \( \varrho^{(0)} \) (2.1), corrections \( u^{(1)} \ll u^{(0)} \) and \( \varrho^{(1)} \ll \varrho^{(0)} \) to the leading-order solution could be found. In a future paper, [8], we present the results of fourth-order accurate calculations, using another model of a diatomic lattice in which, as well as second-neighbour interactions, the interactions of each lattice site with its nearest-neighbours are treated explicitly, as in [9].

References