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Quasi-continuum approximations to lattice equations arising from the discrete nonlinear telegraph equation

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Abstract. We show how quasi-continuum methods can be used to construct approximate solutions of nonlinear differential delay equations derived from symmetry reductions of the discrete nonlinear telegraph equation. Travelling wave solutions are proven to exist and the existence of solutions to two other symmetry reductions are studied. Two of the less familiar reductions are studied; the first supports both a one-parameter family of single-pulse solitary-wave-type solutions and a one-parameter family of periodic waves. The size and shape of these waves are examined using the quasi-continuum technique; this approximates the differential-difference equation with a higher-order differential equation, which is integrated and analysed using phase plane techniques. In the large-amplitude limit, the shape of the pulse approaches a limiting form which has a corner at its peak. The manner of this approach is elucidated using matched asymptotic expansions. The second reduction, though differing only by the addition of a single term, appears not to support the solitary-wave type of solution—even in the limit where the additional term is premultiplied by an asymptotically small constant.

1. Introduction

In [10] Ody *et al* analyse a transmission line composed of inductors (with inductance L) and capacitors (with voltage-dependent capacitance $C(V)$). Denoting the electrical potential (voltage) at the n th node by $u_n(t)$, the governing equation

$$L \frac{d}{dt} \left[C(u_n) \frac{du_n}{dt} \right] = u_{n+1} - 2u_n + u_{n-1} \quad (1.1)$$

is derived. Ody *et al* then investigate the types of solutions supportable by the system through seeking symmetry reductions of this system of equations. In this paper we analyse these reductions in more detail, using quasi-continuum approximations. The relevant theory of electrical transmission lines is reviewed by Remoissenet [11].

One reduction leads to travelling waves ($u_n(t) = u(n - ct) = u(z)$), whose form satisfies a nonlinear differential delay equation; whilst other reductions also lead to differential delay equations. Here, we concentrate on the latter, more general reductions and show how analytical methods designed for travelling wave equations can also be applied to a new scenario, yielding both rigorous information on the existence of certain types of solutions, and approximations to their shape.

We concentrate on the reductions from (1.1) to

$$\text{case A: } a^2 \left(w(z) \frac{d^2 w}{dz^2} - 2 \left(\frac{dw}{dz} \right)^2 \right) = \frac{1}{3} w^3 \delta^2 w(z)^3 \quad (1.2)$$

$$\text{case B: } a^2 \left(w(z) \frac{d^2 w}{dz^2} - 2 \left(\frac{dw}{dz} \right)^2 \right) = w(z)^2 + \frac{1}{3} w^3 \delta^2 w(z)^3 \quad (1.3)$$

where $\delta^2 f(z) = f(z+1) - 2f(z) + f(z-1)$ is the central second-difference operator, and a is a parameter. These reductions arise from $LC(u) = u^{-4/3}$, where $z = x + a/t$ and $u = w^3/t^3$, which leads to case A; and, $z = x - a \tan^{-1} t$ and $u = w^3/(t^2 + 1)^{3/2}$, which leads to case B. In both of these cases the substitution $\phi(z) = 3^{1/4} a^{1/2}/w(z)$ simplifies the problem. In the former equation, this completely removes the parameter a from the problem. We shall thus study the problems in the form:

$$\text{case A: } \frac{d^2 \phi}{dz^2} + \delta^2 \left(\frac{1}{\phi(z)^3} \right) = 0 \quad (1.4)$$

$$\text{case B: } \frac{d^2 \phi}{dz^2} + \delta^2 \left(\frac{1}{\phi(z)^3} \right) + \frac{\phi(z)}{a^2} = 0. \quad (1.5)$$

Formally, case A corresponds to the $a \rightarrow \infty$ limit of case B, and one might thus expect solutions of case B to yield leading-order approximations to solutions of case A in the limit $a \rightarrow \infty$; however, this is not the case. We show that case A supports both periodic-wave solutions and solitary-wave solutions, but that case B cannot support solitary waves; however, a small-amplitude analysis suggests that periodic solutions may exist.

The theorem proved by Friesecke and Wattis [9] rigorously establishes the existence of solitary travelling wave solutions to (1.1) and of more general single-pulse solutions of case A (1.2). These results are detailed in section 2, along with the non-existence of single-pulse and periodic solutions to case B (1.3). The approximate solutions of case A are detailed in section 3, where approximate forms for both solitary and periodic waves are constructed. The paper concludes with a discussion of the results.

The other reductions considered by Ody *et al* in [10] yield equations which are not amenable to quasi-continuum analysis, so these equations are not considered further here. This paper illustrates this fact in that case A is more amenable to quasi-continuum techniques than case B, since higher-order approximations to case A can be reduced to second-order ordinary differential equations than for case B (although this property is somewhat overshadowed and complicated by the fact that case B does not possess solitary-wave solutions, whilst case A does).

1.1. The quasi-continuum method

The second difference operator defined after equation (1.3) makes rigorous and accurate mathematical analysis difficult due to its non-local form. Approximate equations can be gained by replacing it with a local derivative operator; in the simplest and crudest approximation it is replaced by a second derivative. The quasi-continuum approximation technique makes use of higher-order derivatives to form more accurate approximations of the discrete difference operator via Padé approximants. These techniques were developed in [2, 14] to find approximate solutions to differential delay equations arising in the study of solitary waves on lattices (for example, the Fermi–Pasta–Ulam (FPU) lattice [6]†). They are

† The work was actually carried out in Los Alamos in 1959 and initially only written up as an internal report.

generalizations of a technique used by Rosenau [13], which replaced the system of ordinary differential equations by a single partial differential equation, and have since been widely applied to more general systems involving multiple delays and advances [16], and systems with on-site potentials [17].

Formally, the technique replaces a discrete-difference operator with a high-order differential operator, using the identity

$$\delta^2 = \exp(\partial_z) - 2 + \exp(-\partial_z) \tag{1.6}$$

one finds

$$\delta^2 = \partial_z^2 + \frac{1}{12}\partial_z^4 + \frac{1}{360}\partial_z^6 + \dots \tag{1.7}$$

The simplest continuum approximation corresponds to the (2, 0) Padé approximation ($\delta^2 \simeq \partial_z^2$). However, in many cases the (4, 0), the (2, 2) and even the (4, 2) approximates are solvable and give more accurate solutions. These correspond to replacing the second-difference operator with

$$\left(1 + \frac{1}{12}\partial_z^2\right)\partial_z^2 \quad \left(1 - \frac{1}{12}\partial_z^2\right)^{-1}\partial_z^2 \quad \left(1 - \frac{1}{30}\partial_z^2\right)^{-1}\left(1 + \frac{1}{20}\partial_z^2\right)\partial_z^2 \tag{1.8}$$

respectively. In the subsequent sections we concentrate on solving the differential equations resulting from the application of these approximate operators (1.8). See [14] for further details of the approximation process and an analysis of its accuracy.

All the ensuing approximations that we analyse in detail are second-order autonomous ordinary differential equations of the form $\phi''(z) = F(\phi(z), \phi'(z))$, and are thus amenable to phase plane techniques. The exploitation of these geometric techniques requires the replacement of the single equation with a pair of first-order equations ($\phi' = \chi, \chi' = F(\phi, \chi)$), and then equilibrium points to be found (where $\phi' = 0 = \chi'$). In our case, these points correspond to constant solutions $\phi(z) = \phi_c$ satisfying $F(\phi_c, 0) = 0$. A study of the linearized system near these points yields information concerning the structure of phase space. In the examples studied below these fall into one of two categories: (a) centres, in which trajectories close to the stationary point $\phi(t) = \phi_c$ form closed curves in phase space ($\phi'(z)$ versus $\phi(z)$), which correspond to periodic oscillations in $\phi(z)$; and, (b) saddles, where there is an unstable and a stable direction. A saddle point in phase space will generate a solitary wave in $\phi(z)$ if the unstable manifold meets the stable manifold smoothly, in the examples studied here this property can be verified. Since our system is Hamiltonian, it conserves energy; the approximation techniques we use maintain this important property, thus an energy integral can be found, $E = E(\phi, \chi) = E(\phi, \phi')$. The trajectories in phase space are then level sets of the energy function, and so it can be proven that the unstable and stable manifolds of a saddle meet smoothly. The energy integral enables the exact location of the homoclinic connection to be determined in (ϕ, ϕ') -space, and hence the problem is reduced to a first-order nonlinear ordinary differential equation ($E(\phi(z), \phi'(z)) = E(\phi_c, 0)$). In (z, ϕ) -space, the homoclinic trajectory corresponds to a solitary wave, which decays to a constant in the limit $z \rightarrow \pm\infty$, where $\phi \rightarrow \phi_c$ and $\chi = \phi' \rightarrow 0$. The amplitude of the wave can be found by solving $E = E(\phi_0, 0)$ with $\phi_0 \neq \phi_c$.

2. Existence results

The existence theorem of Friesecke and Wattis [9] states that the system of ordinary differential equations

$$\frac{d^2\phi_n(t)}{dt^2} = V'(\phi_{n+1}(t)) - 2V'(\phi_n(t)) + V'(\phi_{n-1}(t)) \tag{2.1}$$

supports travelling solitary-wave solutions satisfying the differential delay equation

$$c^2 \phi''(z) = V'(\phi(z+1)) - 2V'(\phi(z)) + V'(\phi(z-1)) \quad (2.2)$$

provided that the nonlinear nearest-neighbour interaction potential $V(\phi)$ satisfies: (a) the ratio $V(\phi)/\phi^2$ increases strictly with $|\phi|$ for all $\phi \in \Lambda$ where $\Lambda = (-\infty, 0) = \mathbb{R}^-$ or $\Lambda = (0, \infty) = \mathbb{R}^+$; and (b)

$$V(\phi) = \frac{1}{2} V''(0) \phi^2 + \varepsilon |\phi|^p + o(\phi^p) \quad \text{as } \phi \in \Lambda \quad \phi \rightarrow 0 \quad (2.3)$$

for some $\varepsilon > 0$, where $V''(0) \geq 0$ and $2 < p < 6$ (although, it is anticipated that the condition $p < 6$ can be relaxed, at the expense of a more technical proof). Supersonic ($c^2 > V''(0)$) solitary waves of single sign then exist ($\phi > 0$ if $\Lambda = \mathbb{R}^+$ and $\phi < 0$ if $\Lambda = \mathbb{R}^-$). If condition (a) holds and (b) fails, then solitary waves exist with potential energies above some threshold ($\int V(\phi(z)) dz > K_0$); if (b) holds as well as (a), then it is known that $K_0 = 0$, and so solitary waves of arbitrarily small size exist. We now apply this result to the lattice equation (1.1) and to the reduction to case A (1.4).

2.1. Travelling wave solutions

The travelling wave solution of (1.1) satisfies

$$c^2 \frac{d}{dz} \left[C(u(z)) \frac{du}{dz} \right] = u(z+1) - 2u(z) + u(z-1) \quad (2.4)$$

which for general functions $C(u)$ can be recast as (2.2) by $\phi = \tilde{C}(u)$, where $\tilde{C}'(u) = C(u)$; then $V'(\phi) = u = \tilde{C}^{-1}(\phi)$ and $V(\phi) = \int_0^\phi \tilde{C}^{-1}(\varphi) d\varphi$. We then need to check that $V(\phi)$ satisfies the conditions of strict monotonicity and (2.3). The condition $V''(0) \geq 0$ implies $C(0) \geq 0$. In the special case where $C(u)$ is given by a simple power law, as in $C(u) = C_0(q+1)u^q$, we find $\tilde{C}(u) = C_0 u^{q+1}$ and $V'(\phi) = u = [\phi/C_0]^{1/(q+1)}$, which implies $V(\phi) = \frac{q+1}{q+2} C_0^{-\frac{1}{q+1}} \phi^{\frac{q+2}{q+1}}$. Thus for the existence theorem to apply, we need $-\frac{4}{5} < q < 0$, although we expect the result to hold for $-1 < q < 0$. Since $V''(0) = 0$, the waves exist for all speeds $c > 0$. In these cases ϕ and hence $u \rightarrow 0$ as $z \rightarrow \pm\infty$. If $q < -1$, as is the case in [10] where $q = -\frac{4}{3}$, the potential energy function is not compatible with decay to zero as $z \rightarrow \pm\infty$.

2.2. Pulse solutions of case A

The existence theorem can also be applied to case A (1.2), proving the existence of a one-parameter family of solutions whose amplitudes lie within certain bounds. The interpretation of parameters differ from that given above, the result being applicable following a reformulation of the problem. We define $\phi(z) = \phi_\infty - \hat{\phi}(z)$, with $\hat{\phi}(z) \rightarrow 0$ as $z \rightarrow \pm\infty$; so that a wave $\phi(z)$ which decays to the constant ϕ_∞ in the limits $z \rightarrow \pm\infty$, and has amplitude $\hat{\phi}(0)$. We define a potential energy function $V(\hat{\phi})$ by

$$V(\hat{\phi}) = \frac{1}{2(\phi_\infty - \hat{\phi})^2} - \frac{\hat{\phi}}{\phi_\infty^3} - \frac{1}{2\phi_\infty^2} \quad (2.5)$$

so that $V''(0) = 3/\phi_\infty^4 > 0$, $p = 3$ and $\varepsilon = 2/\phi_\infty^5$ in (2.3). Then $V(\hat{\phi})/\hat{\phi}^2$ is strictly increasing on $0 \leq \hat{\phi} < \phi_\infty$, over which $V(\hat{\phi})$, and $V'(\hat{\phi})$ vary from zero to $+\infty$. Since a solution to equation (1.2) must be continuous and differentiable, $\hat{\phi}$ cannot stray into the region $\hat{\phi} > \phi_\infty$;

hence the existence theorem guarantees the existence of a one-parameter family of solitary-wave solutions to the problem (2.2) with $c^2 > V''(0) = 3/\phi_\infty^4$. This problem can be rewritten in terms of $\phi(z)$ as

$$c^2 \frac{d^2 \phi}{dz^2} - \delta^2 \left(\frac{1}{\phi(z)^3} \right) = 0. \tag{2.6}$$

Thus we are interested in the existence of a solution with $c^2 = 1$, which requires $\phi_\infty > 3^{1/4}$. The quantity $V(\hat{\phi})/\hat{\phi}^2$ increases monotonically for $\hat{\phi} > 0$ (and not for $\hat{\phi} < 0$), thus solitary waves $\phi(z)$ satisfy $\phi(z) < \phi_\infty$.

3. Form of solutions in case A

Simply approximating the second difference operator by a second derivative (the leading-order expansion of (1.6)), we find

$$\frac{d^2 \phi}{dz^2} + \frac{d^2}{dz^2} \left(\frac{1}{\phi(z)^3} \right) = 0 \tag{3.1}$$

which can be completely integrated to

$$\phi(z) + \frac{1}{\phi(z)^3} = Az + B \tag{3.2}$$

hence ϕ satisfies a quartic equation. It is straightforward to visualize the solution by plotting z as a function of ϕ , ($z = z(\phi)$). This shows that, when $A \neq 0$, there is no solution connecting the limits $z \rightarrow -\infty$ and $z \rightarrow +\infty$ in a continuous manner, as no value of ϕ makes the right-hand side vanish, which is required when $z = -B/A$. There is only the trivial solution $\phi(z) = \phi_B$, which satisfies the case $A = 0, B = \phi_B + 1/\phi_B^3$. Thus it is necessary to use one of the higher-order quasi-continuum expansion methods to find how solutions to case A behave.

In case A, all terms have either a second difference or a second derivative operator acting on them. Since all continuum expansions contain a factor of ∂_z^2 , the approximating equations can always be immediately integrated twice to reduce their order by two. This reduces fourth derivative terms to second derivatives, leading to problems which are amenable to phase plane techniques and, in some cases, complete integration.

3.1. The (4, 0) Padé approximation

In this case we approximate the second difference operator by $\partial_z^2 + \frac{1}{12}\partial_z^4$, yielding

$$\frac{1}{12} \frac{d^2}{dz^2} \left(\frac{1}{\phi(z)^3} \right) + \phi(z) + \left(\frac{1}{\phi(z)^3} \right) = Az + B \tag{3.3}$$

after two integrations with respect to z . We cannot deal with the fully general case, in which both A and B are arbitrary, thus we restrict ourselves to $A = 0$ and describe the form of solutions in this case, leaving B as an arbitrary constant. The substitution $\psi = 1/\phi^3$ yields

$$\frac{1}{12} \frac{d^2 \psi}{dz^2} + \psi(z) + \psi(z)^{-1/3} = B. \tag{3.4}$$

So that in the (ψ, ψ') phase plane there is a critical point at $(\psi_B, 0)$, we assign the constant B by $B = \psi_B + \psi_B^{-1/3}$. This critical point is a saddle if $\psi_B < 3^{-3/4}$ and a centre if $\psi_B > 3^{-3/4}$. Letting $\phi_B = \psi_B^{-1/3}$ we gain the condition for a solitary wave to exist is $0 < \phi_B < 3^{1/4}$, where

$\phi(z) \rightarrow \phi_B$ as $z \rightarrow \pm\infty$. For $\phi_B > 3^{1/4}$, periodic waves which oscillate around $\phi = \phi_B$ exist. As ϕ_B varies over the range $0 < \phi_B < \infty$, $B = \phi_B + \phi_B^{-3}$ covers $B > 4/3^{3/4} \approx 1.755$. Since (3.3) is symmetric under $\phi \mapsto -\phi$, $B \mapsto -B$, the range $B < -4/3^{3/4}$ is covered by $\phi_B < 0$. Thus the range $|B| < 4/3^{3/4}$ is not parametrized by ϕ_B , for these values of B , there are no critical points in the phase plane of (3.4).

3.1.1. Pulse-like solution of the (4, 0) approximation. First, we shall seek solitary pulse-wave solutions to this equation with the property that $\psi \rightarrow \psi_B < 3^{-3/4}$ and $\psi' \rightarrow 0$ as $z \rightarrow \pm\infty$ by substituting $\psi(z) = \psi_B(1 + \theta(z))$, where $\theta(z)$ is subject to the limiting behaviour $\theta(z), \theta'(z) \rightarrow 0$ as $z \rightarrow \pm\infty$. The determining equation for $\theta(z)$ is thus

$$\frac{1}{12} \frac{d^2\theta}{dz^2} + \theta(z) + \frac{1}{\psi_B^{4/3}(1 + \theta(z))^{1/3}} - \psi_B^{-4/3} = 0 \quad (3.5)$$

which can be integrated to

$$\frac{1}{36} \psi_B^{4/3} \left(\frac{d\theta}{dz} \right)^2 = 1 + \frac{2}{3} \theta(z) - (1 + \theta(z))^{2/3} - \frac{1}{3} \psi_B^{4/3} \theta(z)^2 =: F(\theta). \quad (3.6)$$

The left-hand side of this expression is clearly positive, being the product of squared terms; we define the right-hand side of (3.6) to be $F(\theta)$. Thus the only physically relevant values of θ are those which satisfy $F(\theta) \geq 0$. The function $F(\theta)$ has a double zero at $\theta = 0$, with $F(\theta) \rightarrow 0^+$ as $\theta \rightarrow \pm\infty$; a result which is consistent with exponential decay in the tail of the solitary wave. For small θ , $F(\theta) \simeq \frac{1}{9}(1 - 3\psi_B^{4/3})\theta^2$, confirming the need for $\psi_B < 3^{-3/4}$. The amplitude of the solitary wave is also determined by $\theta'(z) = 0$, implying the existence of another root of $F(\theta)$. For large- θ , the quadratic term will dominate, and make $F(\theta)$ negative ($F(\theta) \sim -\frac{1}{3}\psi_B^{4/3}\theta^2$). Since $F(\theta)$ is continuous, there will be some value of θ , which we define as θ_0 where $F(\theta_0) = 0$. Exact values for the amplitude (θ_0) of the solitary-wave solution satisfy

$$1 + \frac{2}{3}\theta_0 - (1 + \theta_0)^{2/3} = \frac{1}{3}\psi_B^{4/3}\theta_0^2 \quad (3.7)$$

which, for small ψ_B , gives either a large positive value for θ_0 or an $\mathcal{O}(1)$ negative value, with asymptotes $\theta_0 \sim 2\psi_B^{-4/3}$ or $\theta_0 \sim -\frac{9}{8}$ as $\psi_B \rightarrow 0$. For values of ψ_B close to $3^{-3/4}$ we find small-amplitude waves, with $\theta_0 \sim 9(1 - 3\psi_B^{4/3})/4$.

3.1.2. Weakly nonlinear solution of the (4, 0) approximation. For small-amplitude solutions, explicit approximate solutions can be found. Expanding (3.6) in powers of θ , assuming θ to be small, we find

$$\frac{1}{4} \psi_B^{4/3} \left(\frac{d\theta}{dz} \right)^2 = (1 - 3\psi_B^{4/3})\theta(z)^2 - \frac{4}{9}\theta(z)^3 \quad (3.8)$$

which is solved by

$$\theta(z) = \frac{9}{4}(1 - 3\psi_B^{4/3}) \operatorname{sech}^2 \left(z \psi_B^{-2/3} \sqrt{1 - 3\psi_B^{4/3}} \right). \quad (3.9)$$

Thus the original problem has a one-parameter family of solutions which can be approximated by $w(z) = 3^{1/4} a^{1/2} \psi(z)^{1/3}$ when $0 < 1 - 3\psi_B^{4/3} \ll 1$, giving

$$w(z) = 3^{1/4} \psi_B^{1/3} \left[1 + \frac{9}{4}(1 - 3\psi_B^{4/3}) \operatorname{sech}^2 \left(z \psi_B^{-2/3} \sqrt{1 - 3\psi_B^{4/3}} \right) \right]^{1/3}. \quad (3.10)$$

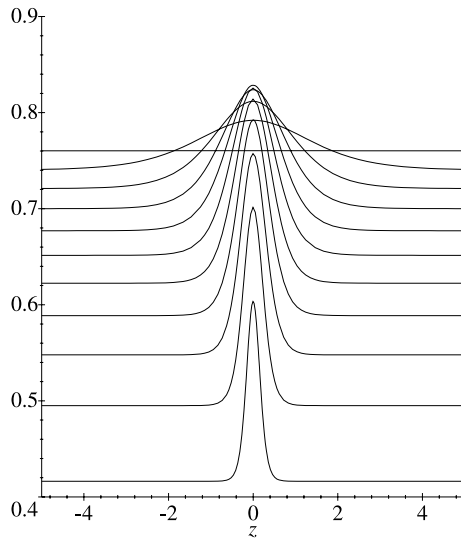


Figure 1. Graphs of the solitary-wave solution (3.10) for $\psi_B^{4/3} = 0.333, 0.3, 0.27, 0.24, 0.21, 0.18, 0.15, 0.12, 0.09, 0.06, 0.03$. The quantity $w(z)/3^{1/4}a^{1/2} = \psi(z)^{1/3} = 1/\phi$ is plotted against z for $-5 < z < 5$ for the value $a = 1$.

3.1.3. *Periodic solutions of the (4, 0) approximation.* For $\psi_B^{4/3} > \frac{1}{3}$, no solitary-wave solution with exponential decay in its tail exists, instead we look for the possibility of periodic solutions. We substitute $\psi(z) = \psi_B(1 + \theta(z))$ into (3.4) with $B = \psi_B + \psi_B^{-1/3}$ to look for solutions which oscillate about $\psi = \psi_B$. Assuming $\theta(z) \ll 1$, a weakly nonlinear expansion produces

$$\frac{1}{12} \frac{d^2\theta}{dz^2} = - \left(1 - \frac{1}{3}\psi_B^{-4/3}\right)\theta(z) - \frac{2}{9}\psi_B^{-4/3}\theta(z)^2. \tag{3.11}$$

Equations of the form $\theta'' = K\theta + L\theta^2$ for $K < 0$ are solved by

$$\theta(z) = \frac{3Km}{2L\sqrt{1-m+m^2}} \left[\text{cn} \left(\frac{z\sqrt{-K}}{2(1-m+m^2)^{1/4}}, m \right)^2 - \left(\frac{2m-1+\sqrt{1-m+m^2}}{3m} \right) \right] \tag{3.12}$$

where cn is the Jacobi elliptic function (see Abramowitz and Stegun [1] for details). This formula (3.12) solves the equivalent first-order problem $\theta'^2 = C + K\theta^2 + \frac{2}{3}L\theta^3$, for any constant C . Hence (3.11) is solved by

$$\theta(z) = \frac{9m(3\psi_B^{4/3}-1)}{4\sqrt{1-m+m^2}} \left[\text{cn}^2 \left(\frac{z\sqrt{3-\psi_B^{-4/3}}}{(1-m+m^2)^{1/4}}, m \right) - \left(\frac{2m-1+\sqrt{1-m+m^2}}{3m} \right) \right]. \tag{3.13}$$

The solution in terms of the original variables, $w(z)$, is then given by $w(z) = 3^{1/4}\psi_B^{1/3}[1 + \theta(z)]^{1/3}$. This solution involves two parameters (m and ψ_B), and has been derived on the basis of the amplitude of oscillation being small, that is $m(3\psi_B^{4/3} - 1) \ll 1$. The solution is sinusoidal for small values of m , but if $(3\psi_B^{4/3} - 1) \ll 1$ then values of m up to unity could also be relevant. These have a longer period and a modified shape, which more closely resembles a train of sech pulses rather than the sinusoidal oscillations which are approached in the limit $m \rightarrow 0$. Such situations are included in figure 2.

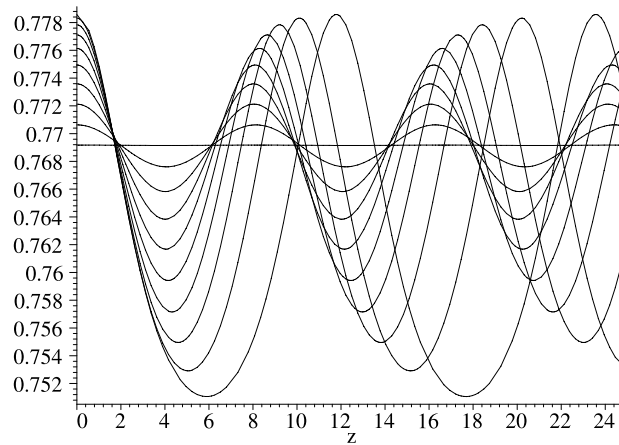


Figure 2. Graphs of the periodic solution derived from (3.13) for $\psi_B^{4/3} = 0.35$, $m = 0.1-0.9$ in steps of 0.1, together with $m = 0.001$. The plot is of $w(z)/3^{1/4}a^{1/2} = 1/\phi = \psi(z)^{1/3} = \psi_B^{1/3}(1+\theta)^{1/3}$ against z for $0 \leq z \leq 25$ in the case $a = 1$.

3.2. The (2, 2) Padé approximation

The (2, 2) Padé approximation (1.8) applied to equation (1.4) yields

$$-\frac{1}{12} \frac{d^2\phi}{dz^2} + \phi(z) + \frac{1}{\phi(z)^3} = Az + B \quad (3.14)$$

after integrating twice with respect to z . We again restrict attention to the case $A = 0$, and use phase plane techniques to analyse the behaviour of the system. The system (3.14) is equivalent to

$$\frac{d\phi}{dz} = \chi \quad \frac{d\chi}{dz} = 12(\phi + \phi^{-3} - B) \quad (3.15)$$

which has a critical point at $\chi = 0$, $\phi = \phi_B$ where $B = \phi_B + \phi_B^{-3}$. The eigenvalues of this point are $\lambda = \pm 2\sqrt{3(1 - 3/\phi_B^4)}$. Thus if $|\phi_B| > 3^{1/4}$ then the critical point is a saddle giving rise to solitary-wave solutions due to the smooth meeting of the unstable and stable manifolds; if $|\phi_B| < 3^{1/4}$ then the critical point is a centre, and we expect to find periodic solutions.

3.2.1. Pulse-like solution of the (2, 2) approximation. Equation (3.14) has a first integral

$$\frac{1}{24} \left(\frac{d\phi}{dz} \right)^2 = \frac{1}{2}\phi(z)^2 - \frac{1}{2}\phi(z)^{-2} - \phi_B\phi(z) - \phi_B^{-3}\phi(z) + \frac{1}{2}\phi_B^2 + \frac{3}{2}\phi_B^{-2} \quad (3.16)$$

where the constant of integration has been set so that $\phi(z) \rightarrow \phi_B$ and $\phi'(z) \rightarrow 0$ as $z \rightarrow \pm\infty$, where $B = \phi_B + \phi_B^{-3}$. To simplify the analysis of such a solitary wave, we transform from $\phi(z)$ to $\theta(z)$ by the substitution $\phi(z) = \phi_B(1 + \theta(z))$, yielding

$$\left(\frac{d\theta}{dz} \right)^2 = \frac{12\theta(z)^2}{\phi_B^4 [1 + \theta(z)]^2} [\phi_B^4\theta(z)^2 + 2\theta(z)(\phi_B^4 - 1) + (\phi_B^4 - 3)] =: F(\theta). \quad (3.17)$$

Now $\theta(z), \theta'(z) \rightarrow 0$ as $z \rightarrow \pm\infty$. Clearly the left-hand side of this expression (3.17) is positive, and thus the right-hand side (i.e. $F(\theta)$) must also be positive. This is satisfied for small θ since $F(0) = 0$, $F'(0) = 0$ and $F''(0) > 0$. However, at the maximum displacement

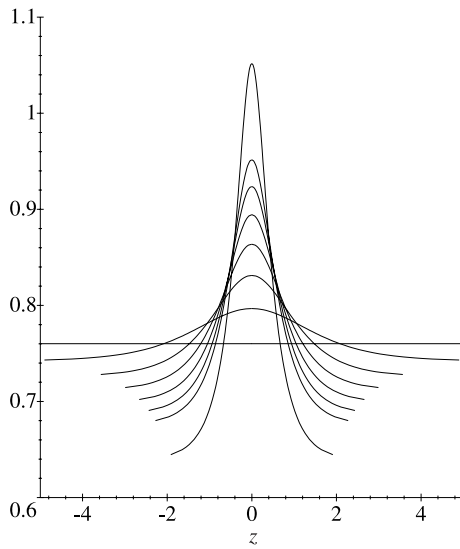


Figure 3. Graphs of the solitary-wave solution (3.19) for $\phi_B^4 = 3, 3.3, 3.6, 3.9, 4.2, 4.5, 4.8, 6$. The quantity $w(z)/3^{1/4}a^{1/2} = 1/\phi(z)$ is plotted against z for $-5 \leq z \leq 5$ in the case $a = 1$.

of the solitary wave which we define as $\theta_0 = \theta(0)$ we must again have $\theta'(0) = 0$ and so $F(\theta_0) = 0$. Thus θ_0 is determined by solving $F(\theta_0) = 0$ with $\theta_0 \neq 0$, which has two negative roots, of which the larger (least negative) determines θ_0 , namely

$$\theta_0 = \phi_B^{-4} - 1 + \phi_B^{-2} \sqrt{1 + \phi_B^{-4}}. \tag{3.18}$$

Solitary waves occupy the region $\theta_0 \leq \theta(z) \leq 0$. Equation (3.17) can be solved implicitly, giving $z = z(\theta)$

$$\begin{aligned} \pm 2\sqrt{3}z(\theta) = \log & \left| \frac{\phi_B^2 \sqrt{\phi_B^4 \theta^2 + 2\theta(\phi_B^4 - 1) + (\phi_B^4 - 3)} + \phi_B^4 \theta + (\phi_B^4 - 1)}{\sqrt{1 + \phi_B^4}} \right| - \frac{\phi_B^2}{\sqrt{\phi_B^4 - 3}} \\ & \times \log \left| \frac{\sqrt{\phi_B^4 - 3} \sqrt{\phi_B^4 \theta^2 + 2\theta(\phi_B^4 - 1) + (\phi_B^4 - 3)} + (\phi_B^4 - 3) + \theta(\phi_B^4 - 1)}{\theta \sqrt{1 + \phi_B^4}} \right| \end{aligned} \tag{3.19}$$

and these curves are plotted in figure 3.

3.2.2. Weakly nonlinear solution of the (2, 2) approximation. When $0 < \phi_B^4 - 3 \ll 1$, the amplitude θ_0 is small and so weakly nonlinear analysis is once again appropriate. We thus neglect $\mathcal{O}(\theta^4)$ terms which reduces equation (3.17) to

$$\left(\frac{d\theta}{dz}\right)^2 = \frac{12\theta(z)^2}{\phi_B^4} [(\phi_B^4 - 3) + 4\theta(z)] \tag{3.20}$$

which can be solved explicitly by

$$\theta(z) = -\frac{1}{4}(\phi_B^4 - 3) \operatorname{sech}^2 \left(z\phi_B^{-2} \sqrt{3(\phi_B^4 - 3)} \right). \tag{3.21}$$

This implies that the solution in our original variables $w(z)$ is given by

$$w(z) = \phi_B^{-1} \left[1 - \frac{1}{4}(\phi_B^4 - 3) \operatorname{sech}^2 \left(z\phi_B^{-2} \sqrt{3(\phi_B^4 - 3)} \right) \right]^{-1} \tag{3.22}$$

which overestimates the amplitude determined by the implicit solution (3.19); however, the errors are vanishingly small in the small-amplitude limit.

3.2.3. Large-amplitude solution of the (2, 2) approximation. We now tackle the harder problem of approximating the more strongly nonlinear problem of finding solitary waves of larger amplitude. We return to the (2, 2) Padé formulation of the problem given in (3.17). For large values of ϕ_B , equation (3.18) implies that the amplitude is given by

$$\theta_0 \sim -1 + \frac{1}{\phi_B^2}. \quad (3.23)$$

It is then possible to find the shape of the solution asymptotically, by rewriting (3.17) as

$$\left(\frac{d\theta}{dz}\right)^2 = 12\theta(z)^2 \left(1 - \frac{3 + 2\theta(z)}{\phi_B^4 [1 + \theta(z)]^2}\right). \quad (3.24)$$

First we examine the ‘inner’ problem, that is the behaviour of the solution near its maximum, by following the scaling for $\theta(z)$ suggested by (3.23) and substituting $\theta(z) = -1 + \varphi(\zeta)/\phi_B^2$ with $\zeta = z_0 z$ where z_0 is to be determined. To leading order in $1/\phi_B^2$ we find

$$\frac{z_0^2}{12\phi_B^4} \left(\frac{d\varphi}{d\zeta}\right)^2 = 1 - \frac{1}{\varphi(z)^2}. \quad (3.25)$$

Thus the natural scaling for the independent variable is $z_0 = 2\sqrt{3}\phi_B^2$, which leads to the inner solution $\varphi(\zeta) = \sqrt{1 + \zeta^2}$. In terms of the outer variable this can be written as

$$\theta(z) = -1 + \frac{\sqrt{1 + 12\phi_B^4 z^2}}{\phi_B^2}. \quad (3.26)$$

To leading order in the outer variables this is $\theta_i(z) = -1 + \sqrt{12}|z|$. Thus in the outer variables, the solitary wave appears to develop a corner as the maximum height of $\theta = -1$ is approached.

We now turn to the ‘outer’ problem, away from the region where $\theta \sim -1$, the leading order determining equation is $(d\theta/dz)^2 = 12\theta^2$, which is solved by $\theta(z) = K \exp(\pm\sqrt{12}z)$ in $z \lesssim 0$ for some constant K . These two solutions match when $K = -1$, since a Taylor expansion of $\theta(z) = -\exp(-\sqrt{12}|z|)$ for small z agrees with the inner solution expanded to terms in the outer variables (the function $\theta_i(z)$ quoted above). In terms of the original variables, the outer solution is

$$w(z) = \frac{1}{\phi(z)} = \frac{\phi_B}{\phi_B^2 - (\phi_B^2 - 1)e^{-|z|\sqrt{12}}}. \quad (3.27)$$

3.2.4. Periodic solutions of the (2, 2) approximation. Finally, in our studies of the (2, 2) Padé approximation, we note the existence of periodic waves when $\phi_B^4 < 3$. In this case we again use the substitution $\phi(z) = \phi_B(1 + \theta(z))$, but now we assume that ϕ oscillates around ϕ_B so that $\theta(z)$ takes both positive and negative values. A small-amplitude expansion of (3.14) gives

$$\frac{1}{12} \frac{d^2\theta}{dz^2} = \theta(z) \left(1 - \frac{3}{\phi_B^4}\right) + \frac{6\theta(z)^2}{\phi_B^4} \quad (3.28)$$

which is solved by the cnoidal wave (see 3.12)

$$\theta(z) = \frac{-m(3 - \phi_B^4)}{4\sqrt{1 - m + m^2}} \left[\text{cn}^2 \left(\frac{z\sqrt{3(3\phi_B^4 - 1)}}{(1 - m + m^2)^{1/4}}, m \right) - \left(\frac{2m - 1 + \sqrt{1 - m + m^2}}{3m} \right) \right]. \quad (3.29)$$

The solution in terms of the original function $w(z)$ is then determined by $w(z) = 1/\phi_B(1+\theta(z))$. Since the solution (3.29) was derived using a weakly nonlinear expansion, it is only valid for small-amplitude waves. However, this does not simply mean small m , where the waves reduce to small perturbations of sinusoidal oscillations. For $0 < 3 - \phi_B^4 \ll 1$, even solutions with larger m will have small amplitude, and thus display a longer time period and non-symmetric oscillation.

3.3. The (4, 2) Padé approximation

Using the last and most accurate approximation from (1.8), our equation reduces to

$$\phi(z) - \frac{1}{30} \frac{d^2\phi}{dz^2} + \frac{1}{\phi(z)^3} + \frac{1}{20} \frac{d^2}{dz^2} \left(\frac{1}{\phi^3} \right) = Az + B \tag{3.30}$$

and, as in all previous analyses, we shall only consider the case $A = 0$. Both the (4, 0) and the (2, 2) Padé approximations correctly handle fourth derivative terms, whereas this approximation also includes the effects of sixth derivative terms correctly. We rewrite the constant B as $\phi_B + 1/\phi_B^3$, so that (3.30) can be rewritten as

$$\frac{1}{60} \frac{d^2\phi}{dz^2} \left(2 + \frac{9}{\phi(z)^4} \right) - \frac{3}{5\phi^5} \left(\frac{d\phi}{dz} \right)^2 + \phi_B - \phi(z) + \frac{1}{\phi_B^3} - \frac{1}{\phi(z)^3} = 0. \tag{3.31}$$

Phase plane techniques then allow us to categorize the system’s behaviour into two cases: for $\phi_B^4 > 3$ we have a saddle point with a homoclinic trajectory joining the stable and unstable manifolds of the saddle point, thus ϕ decays to ϕ_B exponentially in its tail and the homoclinic trajectory corresponds to a single pulse-like solution; when $\phi_B^4 < 3$ there is a periodic wavetrain which oscillates about $\phi = \phi_B$. In both cases the integrating factor $2 + 9/\phi(z)^4$ enables the first integral of (3.30) to be found

$$E = \frac{1}{120} \left(\frac{d\phi}{dz} \right)^2 \left(2 + \frac{9}{\phi(z)^4} \right)^2 - \phi(z)^2 + \frac{11}{2\phi(z)^2} + \frac{3}{2\phi(z)^6} + 2\phi(z) \left(\phi_B + \frac{1}{\phi_B^3} \right) - \frac{3}{\phi(z)^3} \left(\phi_B + \frac{1}{\phi_B^3} \right). \tag{3.32}$$

The problem of finding the shape of the solitary wave or the nonlinear periodic wave now reduces to finding the appropriate value for E and then carrying out quadrature.

3.3.1. Pulse-like solutions of the (4, 2) approximation. Following the techniques adopted in the previous analyses, we substitute $\phi(z) = \phi_B(1 + \theta(z))$, which implies that $\theta, \theta' \rightarrow 0$ as $z \rightarrow \pm\infty$. The critical value for E which generates a solitary-wave solution is found by letting $\phi(z) \rightarrow \phi_B$ and $\phi'(z) \rightarrow 0$ in (3.32) yielding $E = \phi_B^2 + 9/2\phi_B^2 - 3/2\phi_B^6$. With this value of E , equation (3.32) reduces to

$$\begin{aligned} & \frac{1}{120} \left(\frac{d\theta}{dz} \right)^2 \left(2 + \frac{9}{\phi_B^4(1 + \theta(z))^4} \right)^2 \\ &= \theta(z)^2 \left(1 + \frac{3 - 7\theta(z) - 4\theta(z)^2}{2\phi_B^4(1 + \theta(z))^3} - \frac{3(3 + 3\theta(z) + \theta(z)^2)^2}{2\phi_B^8(1 + \theta(z))^6} \right) \\ &=: F(\theta). \end{aligned} \tag{3.33}$$

The next logical stage of the calculation is to find the amplitude of the solitary wave, θ_0 , by solving $F(\theta_0) = 0$; unfortunately this is not possible since it yields a sixth-degree polynomial. $F(\theta_0) = 0$ can, however, be solved implicitly for ϕ_B^4 as a function of θ_0 , giving

$$\phi_B^{-4} = \frac{(1 + \theta_0)^3}{6(3 + 3\theta_0 + \theta_0^2)^2} \left(3 - 7\theta_0 - 4\theta_0^2 + \sqrt{5(45 + 78\theta_0 + 77\theta_0^2 + 40\theta_0^3 + 8\theta_0^4)} \right) \quad (3.34)$$

which can be plotted and shown to give a unique value of θ_0 for each value of $\phi_B > 3^{1/4}$. This enables (3.33) to be rewritten as an integral for $z = z(\theta)$

$$z(\theta) = \frac{\pm \phi_B^4}{2\sqrt{15}} \int_{\theta}^{\theta_0} \frac{[2(1+u)^4 + 9\phi_B^{-4}] du}{u(1+u)\sqrt{2\phi_B^8(1+u)^6 + \phi_B^4(3-7u-4u^2)(1+u)^3 - 3(3+3u+u^2)^2}}. \quad (3.35)$$

3.3.2. Weakly nonlinear solution of the (4, 2) approximation. Although it is not possible to convert (3.35) into an explicit solution, we can find an explicit approximate solution when the nonlinearity plays only a weak role in the behaviour of the system. In this limit, the right-hand side of (3.33) can be replaced by the first two terms of its Taylor series for small θ , which leads to

$$\left(\frac{d\theta}{dz} \right)^2 = \frac{60(\phi_B^4 - 3)\theta^2}{(2\phi_B^4 + 9)} \left[1 + \frac{4\theta(14\phi_B^4 - 27)}{(\phi_B^4 - 3)(2\phi_B^4 + 9)} \right]. \quad (3.36)$$

This equation is solved by

$$\theta(z) = \frac{-(\phi_B^4 - 3)(2\phi_B^4 + 9)}{4(14\phi_B^4 - 27)} \operatorname{sech}^2 \left(z \sqrt{15 \left(\frac{\phi_B^4 - 3}{2\phi_B^4 + 9} \right)} \right). \quad (3.37)$$

Plots of this function for a range of values of ϕ_B are shown in figure 4. Note that the more accurate quasi-continuum approximation has yielded wider, smaller pulses than the other weakly nonlinear solutions (3.9) and (3.22). This solution is closer to the fully nonlinear solution (3.19) of the (2, 2) approximation pictured in figure 3 than the (4, 0) approximate (3.10) graphed in figure 1.

3.3.3. Large-amplitude solution of the (4, 2) Padé approximation. We now turn to tackle the more complex case where the waves are of larger amplitude, and hence suffer stronger nonlinear influences. We consider the large-amplitude limit, where $\phi_B \gg 1$, equation (3.33) implies the amplitude $\theta_0 = \theta(0)$ is determined by

$$\theta_0 \sim -1 + \left(\frac{\sqrt{3}}{\sqrt{3} + \sqrt{5}} \right)^{1/3} \frac{1}{\phi_B^{4/3}}. \quad (3.38)$$

We first study the ‘outer’ problem, adopting the scaling of $\theta(z) = -1 + \mathcal{O}(1)$, we find the leading-order equation $(d\theta/dz)^2 = 30\theta^2$ from (3.33), which has the solution

$$\theta(z) = -\exp\left(-\sqrt{30}(|z| - z_0)\right) \quad (3.39)$$

for some constant $z_0 > 0$ which will be determined later through the procedure of asymptotic matching as in section 3.2.3. The solution (3.39) cannot be globally valid, since it is not differentiable at $z = z_0$, and, whilst θ can approach -1 , it can never equal -1 . We assume that the solution is even ($\psi(-z) = \psi(z)$), and consider its form in $z \geq 0$ only.

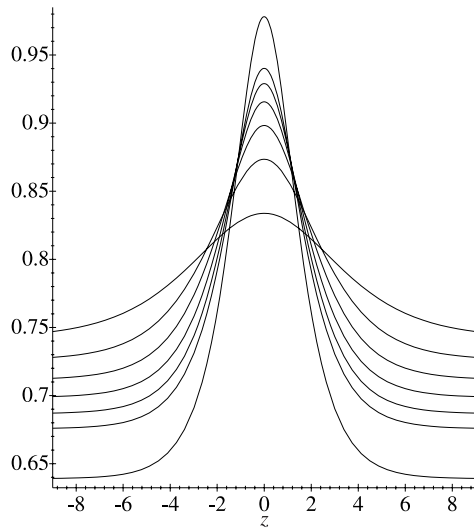


Figure 4. Graphs of the solitary-wave solution (3.37) for $\phi_B^4 = 3.3, 3.6, 3.9, 4.2, 4.5, 4.8, 6$. The quantity $w(z)/3^{1/4}a^{1/2} = 1/\phi(z)$ is plotted against z for $-9 \leq z \leq 9$ in the case $a = 1$.

The solution (3.39) is valid only, whilst θ remains an $\mathcal{O}(1)$ amount above -1 ; as $z \rightarrow z_0^+$ a new ‘intermediate’ region is entered. Expanding (3.39) for small $z - z_0$ we find

$$\theta(z) = -1 + \sqrt{30}(z - z_0) \quad \text{as } z \rightarrow z_0^+ \tag{3.40}$$

so as to match with this, the intermediate region must be defined by $\theta(z) = -1 + \varphi(\zeta)/\phi_B^q$ with $\zeta = z\phi_B^q$. The exponent q is found by balancing terms in (3.33), leading to $q = 1$, and providing the equation

$$\frac{1}{120} \left(\frac{d\varphi}{d\zeta} \right)^2 \left(2 + \frac{9}{\varphi^4} \right)^2 = 1 \tag{3.41}$$

for $\varphi(\zeta)$, which is solved implicitly by $\zeta(\varphi) = \zeta_0 \pm (\varphi - 3/2\varphi^3)/\sqrt{30}$. In terms of the outer variables, this can be written as

$$z(\theta) = z_0 \pm \frac{1}{\sqrt{30}} \left(1 + \theta - \frac{3}{2\phi_B^4(1 + \theta)^3} \right). \tag{3.42}$$

Matching the $1 + \theta \gg 1/\phi_B$ limit of (3.42) to the intermediate limit of the outer solution given in (3.40) enables the constant $\zeta_0 = z_0\phi_B$ to be assigned and the \pm sign to be determined as positive.

Clearly the solution (3.42) moderates the approach of θ to -1 ; however, a third region, which we shall term the ‘inner’ region, is needed to account for the peak of the wave. Taking the limit $\theta \rightarrow -1$ of (3.42), we find that in the matching region between the intermediate region and the inner region we must have

$$\theta = -1 + \left(\frac{\sqrt{3}}{2\sqrt{10}\phi_B^4(z_0 - z)} \right)^{1/3}. \tag{3.43}$$

Following this scaling, which agrees with the expression for the amplitude given in (3.38), we adopt the inner variables $\theta(z) = -1 + \widehat{\varphi}(\widehat{\zeta})/\phi_B^{4/3}$ with $\widehat{\zeta} = z$ and thus derive

$$\frac{27}{40} \left(\frac{d\widehat{\varphi}}{d\widehat{\zeta}} \right)^2 = \widehat{\varphi}^2 \left(\widehat{\varphi}^6 + 3\widehat{\varphi}^3 - \frac{3}{2} \right) \tag{3.44}$$

from (3.33). Again, no explicit solution is available, only the implicit solution

$$\widehat{\zeta}(\widehat{\varphi}) = \sqrt{\frac{27}{40}} \int_{\widehat{\varphi}_0}^{\widehat{\varphi}} \frac{d\widetilde{\varphi}}{\widetilde{\varphi} \sqrt{\widetilde{\varphi}^6 + 3\widetilde{\varphi}^3 - \frac{3}{2}}} \quad (3.45)$$

where $\widetilde{\varphi}_0$ is defined by $\widetilde{\varphi}_0 = (\sqrt{3}/(\sqrt{3}+\sqrt{5}))^{1/3}$ from (3.38). The solution (3.45) has a smooth peak, as can be seen by taking the limit $\widehat{\varphi} \rightarrow \widehat{\varphi}_0$. The solution (3.45) also matches to (3.43) as $\widehat{\varphi} \rightarrow +\infty$, since

$$\widehat{\zeta} \sim \widehat{\zeta}_0 - \frac{\sqrt{3}}{2\sqrt{10}\widehat{\varphi}^3} \quad \text{as } \widehat{\varphi} \rightarrow \infty \quad (3.46)$$

where

$$\widehat{\zeta}_0 = \left(3\sqrt{3}/2\sqrt{10}\right) \int_{\widehat{\varphi}_0}^{\infty} \frac{d\widetilde{\varphi}}{\widetilde{\varphi} \sqrt{\widetilde{\varphi}^6 + 3\widetilde{\varphi}^3 - \frac{3}{2}}}$$

which Maple evaluates as approximately 0.5493. Rewriting (3.46) in terms of the outer variables yields (3.43) along with $z_0 = \widehat{\zeta}_0$.

To summarize, the inner solution shows that the peak of the wave is differentiable and has a zero derivative. The intermediate region shows that the width of the pulse is approximately $2z_0 \approx 1.10$, as one would expect in a lattice equation where the nodes are spaced at unit intervals. The outer solution shows exponential relaxation to the stable equilibrium solution of $\phi = \phi_B$. Thus the method of matched asymptotic expansions enables us to approximate the form of large-amplitude pulse solution for the (4, 2) Padé approximation, however, the added accuracy of this approximation has the cost of a more complicated asymptotic structure than the (2, 2) Padé approximation analysed earlier.

3.3.4. Periodic solutions of the (4, 2) approximation. In the case $\phi_B^4 < 3$, substitution of $\phi(z) = \phi_B(1 + \theta(z))$ into (3.31) followed by an expansion for small θ leads to the equation

$$\begin{aligned} \frac{E}{\phi_B^2} - \left(1 + \frac{9}{2\phi_B^4} - \frac{3}{2\phi_B^2}\right) &= \frac{1}{120} \left(\frac{d\theta}{dz}\right)^2 \left(2 + \frac{9}{\phi_B^4}\right)^2 \left(1 - \frac{72\theta(z)}{2\phi_B^4 + 9}\right) \\ &+ \frac{\theta(z)^2}{2} \left(2 + \frac{9}{\phi_B^4}\right) \left(\frac{3}{\phi_B^4} - 1\right) + \frac{2\theta(z)^3}{\phi_B^4} \left(4 - \frac{27}{\phi_B^4}\right) \end{aligned} \quad (3.47)$$

where E is a constant of integration. For small-amplitude disturbances $\theta(z)$, this formula has the form $\widetilde{E} = \theta'^2 + \omega^2\theta^2$, for some constant of integration \widetilde{E} , indicating the existence of periodic solutions. However, for larger-amplitude oscillations, correction terms of the form $\theta'^2\theta$ as well as θ^3 are introduced. In previous approximations only the latter has appeared, leading to waves which can be expressed in terms of the Jacobi cnoidal function. The additional $\theta'^2\theta$ term complicates the equation to an extent where it is not possible to write down an explicit solution even in the weakly nonlinear case. At small amplitude, the periodic oscillations $\theta \propto \cos(\omega z)$ have frequency given by

$$\omega = 2\sqrt{\frac{15(3 - \phi_B^4)}{2\phi_B^4 + 9}}. \quad (3.48)$$

Thus in this section we have seen that the quasi-continuum approximation method produces a sequence of approximate solutions for the equation referred to as case A in (1.4). These approximate solutions are consistent in form, all producing periodic solutions in the case $\phi_B^4 < 3$ and single-pulse solitary waves in the case $\phi_B^4 > 3$.

3.3.5. *Higher-order approximations.* Even higher-order Padé approximants could be used, but lead to higher-order differential equations, which cannot be analysed to the same level. For example, in case A, the (6, 0), (4, 2) and (2, 4) Padé approximants yield the fourth-order equations

$$\frac{1}{360} \frac{d^4}{dz^4} \left(\frac{1}{\phi^3} \right) + \frac{1}{12} \frac{d^2}{dz^2} \left(\frac{1}{\phi^3} \right) + \frac{1}{\phi^3} + \phi = Az + B \tag{3.49}$$

$$\frac{13}{10080} \frac{d^4}{dz^4} \left(\frac{1}{\phi^3} \right) + \frac{d^2}{dz^2} \left(\frac{11}{168\phi^3} - \frac{\phi}{56} \right) + \phi + \frac{1}{\phi^3} = Az + B \tag{3.50}$$

$$\frac{1}{240} \frac{d^4\phi}{dz^4} - \frac{1}{12} \frac{d^2\phi}{dz^2} + \phi + \frac{1}{\phi^3} = Az + B \tag{3.51}$$

in which the existence of the homoclinic connection is not easy to demonstrate since the phase space is now four dimensional. Yet such a detailed analysis is essential to gain information on the single-pulse solitary-wave solution.

4. Case B

We turn now to case B and again seek single-pulse solutions and periodic-wave solutions using continuum methods to generate approximate solutions. The simplest continuum approximation replaces the second difference operator by a second derivative to yield

$$\frac{d^2\phi}{dz^2} \left(1 - \frac{3}{\phi(z)^4} \right) + \frac{12}{\phi(z)^5} \left(\frac{d\phi}{dz} \right)^2 + \frac{\phi}{a^2} = 0. \tag{4.1}$$

However, let us first analyse the differential-difference equation (1.5); we assume the existence of a single-pulse solution of the form $\phi(z) = \phi_\infty + \psi(z)$ with $\psi(z), \psi'(z) \rightarrow 0$ as $z \rightarrow \pm\infty$. In this limit, and for $\phi_\infty \neq 0$, equation (1.5) leads to

$$\frac{\phi_\infty}{a^2} + \frac{\psi(z)}{a^2} + \psi''(z) + \delta^2 \left(\frac{-3\psi(z)}{\phi_\infty^4} \right) = 0. \tag{4.2}$$

By considering $z \rightarrow \pm\infty$, we see that there is no non-zero value of ϕ_∞ which satisfies (4.2). Thus if a single-pulse solution exists it must satisfy $\phi(z) \rightarrow 0$ as $z \rightarrow \pm\infty$. For special, isolated values of the parameter a , it is possible to find an exact explicit solution for (1.5) in the form of a single pulse. We return to the formulation given in (1.3), and note that a pulse satisfying $\phi(z) \rightarrow 0$ as $z \rightarrow \pm\infty$ corresponds to a solution in which $w(z) \rightarrow \infty$ as $z \rightarrow \pm\infty$. If we assume that a solution grows according to a power law, $w(z) \sim w_0 z^n$ as $z \rightarrow \infty$, then the only value of n which balances all the terms in (1.3) as $z \rightarrow \infty$ is $n = 2$. Since the equation is invariant under translations in z ($z \mapsto z+z_0$), we assume a solution of the form $w(z) = Az^2 + C$, leading to $A = -\frac{1}{10}, C = \frac{1}{8}(6a^2 - 1)$; equation (1.3) is then satisfied only if the parameter a is a root of $7 - 120a^2 + 450a^4 = 0$, yielding $a^2 = \frac{1}{30}[4 \pm \sqrt{2}] \approx 0.18047, 0.08619$. For these special values of a , we have the explicit approximate solutions

$$w(z) = -\frac{1}{10}(z - z_0)^2 - \frac{1}{40}(\sqrt{2} + 1) \quad \text{if } a^2 = \frac{1}{30}(4 - \sqrt{2}) \tag{4.3}$$

$$w(z) = -\frac{1}{10}(z - z_0)^2 + \frac{1}{40}(\sqrt{2} - 1) \quad \text{if } a^2 = \frac{1}{30}(4 + \sqrt{2}) \tag{4.4}$$

valid in the large $z - z_0$ regions. Only the first of these two is well defined in the ϕ -formulation of the problem, since the latter contains divergences at $z - z_0 = \pm \frac{1}{2}\sqrt{1 + \sqrt{2}}$ where $w(z) = 0$. In terms of $\phi(z)$, the former's shape is that of a single pulse which decays according to $\phi(z) \sim z^{-2}$ as $z \rightarrow \pm\infty$.

Considering now the simplest continuum approximation (4.1) with the assumption $\phi(z) \rightarrow \phi_B$ as $z \rightarrow \pm\infty$, we immediately find $\phi_B = 0$. In this case, (4.1) can be integrated to

$$\frac{a^2}{2} \left(\frac{d\phi}{dz} \right)^2 \left(1 - \frac{3}{\phi(z)^4} \right)^2 = E - \frac{1}{2}\phi(z)^2 - \frac{3}{2}\phi(z)^{-2} \quad (4.5)$$

for some constant of integration, E . Whatever value of E is chosen, a contradiction becomes apparent in the limit $z \rightarrow \infty$, since in this limit $\phi \rightarrow 0$ so the right-hand side is negative, whereas the left-hand side must be positive since it is the product of squared terms. Thus no pulse-type solution can exist in this continuum approximation of case B.

We turn now to the possible existence of nonlinear periodic-wave solutions of (4.1). Since any such solution must also solve (4.5) we look for the maximum ($\phi = \phi_+$) and minimum ($\phi = \phi_-$) values of a solution by putting $d\phi/dz = 0$ in (4.5). This implies that ϕ_{\pm} both satisfy the equation

$$0 = \phi^4 - 2E\phi^2 + 3. \quad (4.6)$$

This quadratic has two real roots ($\phi_{\pm}^2 = E \pm \sqrt{E^2 - 3}$), thus for $E > \sqrt{3}$ there are real distinct non-zero values for ϕ_{\pm} . In particular, if put $E = \sqrt{3}(1 + \varepsilon)$ with $\varepsilon \ll 1$, we find $\phi_{\pm}^2 = \sqrt{3}(1 \pm \sqrt{2\varepsilon})$. This suggests the presence of oscillations around $\phi(z) = \pm 3^{1/4}$, with $\phi_+ = \sqrt{\sqrt{3}(1 + \sqrt{2\varepsilon})}$ and $\phi_- = \sqrt{\sqrt{3}(1 - \sqrt{2\varepsilon})}$, hence we substitute $\phi = \pm 3^{1/4}(1 + \theta(z))$ with $\theta = \mathcal{O}(\varepsilon^{1/2})$. When $\phi(z) = \pm 3^{1/4}$, both the coefficient of $\phi'(z)^2$ in (4.5) and the coefficient of $\phi''(z)$ in (4.1) vanish, suggesting that oscillations around these points do not have the usual sinusoidal shape that one would expect from a leading-order small-amplitude expansion. Instead, at leading order we find $\varepsilon = 2\theta^2 + 8a^2\theta^2(\theta')^2$, whose solution is

$$\theta(z) = \pm \sqrt{\frac{2a^2\varepsilon - (z - z_0)^2}{4a^2}}. \quad (4.7)$$

Positive and negative sections of this solution can be pieced together to form an oscillatory solution whose gradient diverges in the limit $\theta \rightarrow 0$ (that is, at $z - z_0 = \pm a\sqrt{2\varepsilon}$).

$$\theta(z) = \begin{cases} \sqrt{\frac{2a^2\varepsilon - (z - z_0 - 4an\sqrt{2\varepsilon})^2}{4a^2}} & \text{if } (4n - 1)a\sqrt{2\varepsilon} < z - z_0 < (4n + 1)a\sqrt{2\varepsilon} & \text{for some } n \in \mathbb{Z} \\ -\sqrt{\frac{2a^2\varepsilon - (z - z_0 - a(4n + 2)\sqrt{2\varepsilon})^2}{4a^2}} & \text{if } (4n + 1)a\sqrt{2\varepsilon} < z - z_0 < (4n + 3)a\sqrt{2\varepsilon} & \text{for some } n \in \mathbb{Z}. \end{cases} \quad (4.8)$$

5. Conclusions

We have been able to analyse case A (1.2) using a variety of approximation techniques. The standard continuum approximation yields no solution on the whole of $z \in \mathbb{R}$. A similar result was found when analysing case B (1.3) using the standard continuum approximation, namely that no solution to the equation could be found. When higher-order continuum approximations are applied to case B, its structure leads to more complicated approximating equations than case A, since the resulting differential equations are of higher order than case A, and cannot be solved explicitly.

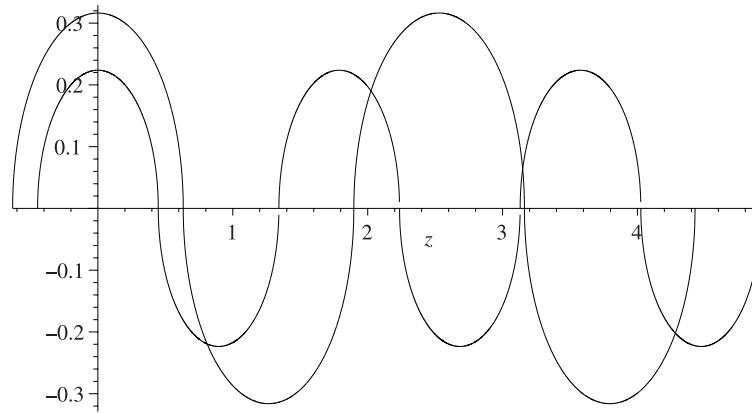


Figure 5. Graphs of the periodic-wave solution (from equation(4.8)) for case B; $\theta(z)$ is plotted against z for $a = 1$, the larger-amplitude oscillation corresponding to $\varepsilon = 0.2$, and the smaller to $\varepsilon = 0.1$.

Higher-order approximations of case B can be derived by using more accurate Padé approximations to the second central difference, such as those quoted in (1.8) which generate the (4, 0), the (2, 2) and the (4, 2) Padé approximate equations

$$0 = \frac{\phi}{a^2} + \frac{d^2}{dz^2} \left(\phi + \frac{1}{\phi^3} \right) + \frac{1}{12} \frac{d^4}{dz^4} \left(\frac{1}{\phi^3} \right) \tag{5.1}$$

$$0 = \frac{\phi}{a^2} + \frac{d^2}{dz^2} \left(\phi + \frac{1}{\phi^3} \right) - \frac{1}{12a^2} \frac{d^2\phi}{dz^2} - \frac{1}{12} \frac{d^4\phi}{dz^4} \tag{5.2}$$

$$0 = \frac{\phi}{a^2} + \frac{d^2}{dz^2} \left(\phi + \frac{1}{\phi^3} \right) + \frac{1}{20} \frac{d^4}{dz^4} \left(\frac{1}{\phi^3} \right) - \frac{1}{30a^2} \frac{d^2\phi}{dz^2} - \frac{1}{30} \frac{d^4\phi}{dz^4} \tag{5.3}$$

respectively. Unfortunately it has so far proved impossible to make analytical progress with these equations, since they are all fourth-order ordinary differential equations. However, direct asymptotic analysis of case B has yielded a non-existence result for solitary-wave solutions for general values of the parameter a . Hence it is unlikely that quasicontinuum approximations will yield solitary-wave solutions. More accurate periodic-wave solutions may be obtainable from (5.1)–(5.3), and it is expected that in the limit $a \gg 1$, the periodic-wave solutions of cases A and B would be similar.

The more advanced, quasi-continuum approximation techniques are effective in case A, and when one of the constants of integration is set to zero, solutions can be found. These are explicit solutions in the case of weak nonlinearity and implicit solutions for the more general cases of arbitrary nonlinearity. These methods include higher derivatives which account for the discreteness and yield both pulse-type solitary-wave and periodic-wave solutions to the equation. The most accurate quasi-continuum approximation (the (4, 2) Padé) yields broadly similar results to the two simpler approximations (the (2, 2) and (4, 0) Padé). All three of the higher-order quasi-continuum approximations yield a second-order autonomous system, which can always be integrated to give the solution implicitly. Thus quasi-continuum approximations are useful in illustrating the form of solutions in cases where a simple continuum limit produces an insoluble equation.

Our results show that there is a critical value of the constant of integration B , namely 2, below which there are no non-trivial solutions. For values of B greater than 2, phase

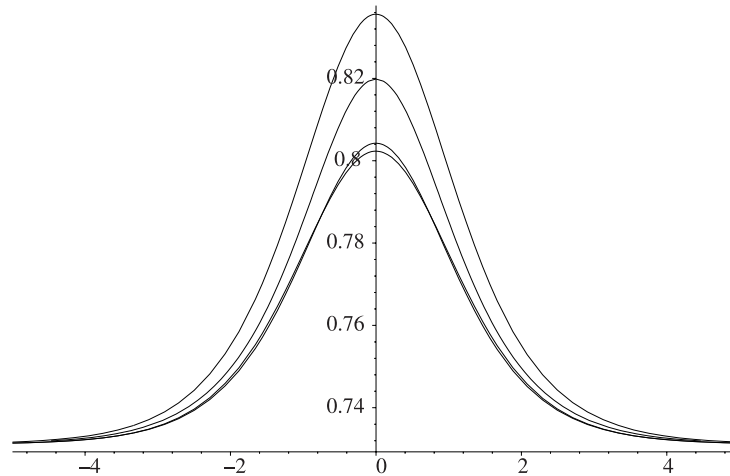


Figure 6. Graphs of the function $w(z)/3^{1/4}a^{1/2}$ against z , for the case $a = 1$, $\phi_B = 3.5^{1/4}$. In increasing amplitude, the curves are the weakly nonlinear (4, 0) approximation (3.10), the weakly nonlinear (4, 2) approximation (3.37), the full (2, 2) approximation (3.19) and the weakly nonlinear (2, 2) approximation (3.22).

plane analysis shows the existence of two critical points, one of which is a centre and the other a saddle. Periodic solutions correspond to oscillations around the centre, and there is a saddle with a homoclinic connection corresponding to a pulse-type solitary-wave solution. Our analysis has concentrated on the two cases $\phi_B < 3^{1/4}$ and $\phi_B > 3^{1/4}$ separately, where $B = \phi_B + \phi_B^{-3}$. Yet for any given value of B , there are two values of ϕ_B satisfying this equation, one lying either side of $3^{1/4}$. Thus the centre and saddle exist in the same system, as illustrated in figure 7.

A comparison of the various methods is shown in figure 6. This shows that the largest-amplitude approximation is the weakly nonlinear (2, 2) Padé approximation (3.22); the smallest-amplitude waves are the weakly nonlinear (4, 0) Padé and (4, 2) Padé approximations, (equations (3.10) and (3.37), respectively). Of these two, although the (4, 2) Padé is slightly larger, the (4, 0) Padé is slightly wider. Between the three weakly nonlinear solutions is the full (2, 2) Padé approximation, which we expect to be more accurate, since it accounts for the full nonlinearity. Comparison with numerical work has been made previously, Eilbeck and Flesch [5] have constructed sophisticated numerical solutions to such differential delay equations in the past, and quasi-continuum approximations tested against them demonstrating the accuracy of the method [14]. The ability to resolve subtle, higher-order, effects has also been reported, for example anisotropy in multi-dimensional lattices, where numerical work of Eilbeck [4] can be compared with quasi-continuum results [15].

The existence of solutions to quasi-continuum approximations does not rigorously prove the existence of solutions to the original system, but they do give a strong indication of the form of solutions assuming existence. They are thus useful for providing initial estimates for numerical schemes should a highly accurate numerical solution of the equations be desired. Rigorous existence results are available [9], and we have modified these results to show how they may be applied to the cases under consideration here. We have not addressed the stability of the waves, but numerical work on travelling waves in FPU lattices suggest they are stable [7]. The rigorous work of [9] is currently being extended by Friesecke and Pego [8] with the aim of analysing stability. These methods rely on the variational formulation of the problem,

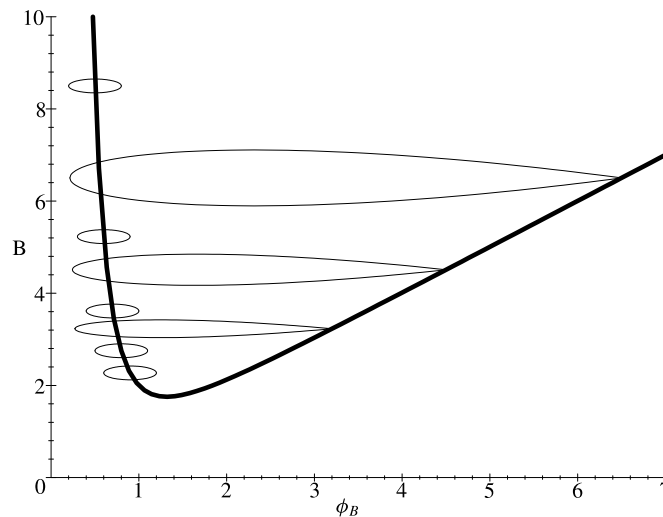


Figure 7. Graphs of the constant $B = \phi_B + \phi_B^{-3}$ against the position of critical point ϕ_B (thick curve); indicating that when $\phi_B < 3^{1/4} \approx 1.3$ the critical point at $\phi = \phi_B$ is a centre and has periodic trajectories encircling it; and when $\phi_B > 3^{1/4}$ the critical point at $\phi = \phi_B$ is a saddle with a homoclinic connection which encircles the other solution of $B = \phi_B + \phi_B^{-3}$.

which can itself be used to generate approximate solutions; see, for example, Duncan and Wattis [3] for details.

Our large-amplitude asymptotic approximations to solitary waves have elucidated the approach of solitary waves to a limiting form which has a corner at the wave's peak. This behaviour has been noted before, most famously in the Stokes waves of maximum amplitude [18], but also in similar lattice systems, for example, the experimental electrical transmission lattice of Remoissenet and Michaux [12] for which solitary waves with corners have been calculated numerically by Eilbeck [4]. We have constructed matched asymptotic expansions of the waves in this strongly nonlinear regime, and so elucidated the manner in which this special solution is approached.

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