

Emergence of unsteady dark solitary waves from coalescing spatially-periodic patterns

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A dark solitary wave, in one space dimension and time, is a wave which is biasymptotic to a periodic state, with a phase shift, and with localized modulation in between. The most well known case of dark solitary waves is the exact solution of the defocussing nonlinear Schrödinger equation. In this paper the interest is in a mechanism for the emergence of dark solitary waves in general, not necessarily integrable, Hamiltonian PDEs. The focus is on the periodic state at infinity as the generator. It is shown that a natural mechanism for the emergence is a transition between one periodic state which is (spatially) elliptic and one which is (spatially) hyperbolic. It is shown that the emergence is governed by a Korteweg-de Vries (KdV) equation for the perturbation wavenumber on a periodic background. A novelty in the result is that the three coefficients in the KdV equation are determined by the Krein signature of the elliptic periodic orbit, the curvature of the wave action flux, and the slope of the wave action, with the latter two evaluated at the critical periodic state.

Key words: nonlinear waves, Hamiltonian systems, solitary waves.

1. Introduction

Dark solitary waves (DSWs) are waves that are biasymptotic to a periodic state, with modulation in between. They are most well known as exact solutions of the defocussing nonlinear Schrödinger (NLS) equation,

$$iA_t + A_{xx} - |A|^2 A = 0, \quad (1.1)$$

for the complex-valued function $A(x, t)$. An example DSW solution is

$$A(x, t) = \sqrt{2}e^{i(kx - \omega t)} [k + i\beta \tanh(\beta x)]. \quad (1.2)$$

where $\beta^2 = \frac{1}{2}(\omega - 3k^2)$ with $\omega > 0$. With ω fixed, the above family of DSWs is a one-parameter family parameterized by k , bi-asymptotic to a spatially periodic state, with

$$\lim_{|x| \rightarrow \infty} |A(x, t)| = 2(k^2 + \beta^2) = \omega - k^2.$$

The background spatially periodic state exists for $-\sqrt{\omega} < k < \sqrt{\omega}$. The DSW emerges when $3k^2 = \omega$ and it exists in the narrower band $-\sqrt{\omega/3} < k < \sqrt{\omega/3}$.

The purpose of this paper is to develop a theory for this emergence of a DSW from a spatially periodic state. The main interest is in a theory for this phenomena in Hamiltonian PDEs that are not in general integrable. However, an idea of the

mechanism that leads to emergence can be clearly seen by considering the case of defocussing NLS.

The first theory for the emergence of DSWs was proposed by KIVSHAR (1990). Kivshar's theory starts with defocussing NLS and proposes a perturbation

$$A(x, t) = [\hat{A} + \varepsilon^2 u(X, T, \varepsilon)] e^{i(kx - \omega t + \varepsilon \phi(X, T, \varepsilon))}.$$

where

$$X = \varepsilon x \quad \text{and} \quad T = \varepsilon^3 t. \quad (1.3)$$

Expanding ϕ and u in a perturbation series in ε and imposing a solvability condition leads to a Korteweg-de Vries (KdV) equation for the leading order term u_1 ,

$$a_0 \frac{\partial u_1}{\partial T} + a_1 u_1 \frac{\partial u_1}{\partial X} + a_2 \frac{\partial^3 u_1}{\partial X^3} = 0,$$

where the coefficients a_0 , a_1 and a_2 depend on (ω, k) ; that is, the emergence of DSWs is governed by a KdV equation. This theory is extended by KIVSHAR ET AL. (1993) to the non-integrable NLS where the cubic nonlinearity is replaced by a general nonlinearity $f(|A|^2)A$. A validity proof of the reduction NLS \rightarrow KdV for the general nonlinearity is proved by CHIRON & ROUSSET (2010) (see also BÉTHUEL ET AL. 2009, 2010). Moreover, they extend the theory to defocussing NLS in two-space dimensions in which case the reduction is NLS to KP-I.

One feature that is hidden in this theory is the bifurcation that the spatially periodic state must undergo in order to generate the KdV equation. The fact that there must be a bifurcation is clear since the generic modulation of a spatially periodic state (or spatially periodic travelling wave) is governed by the Whitham modulation equations which are dispersionless. Indeed DÜLL & SCHNEIDER (2009) prove that the dispersionless Whitham equations are the valid modulation equation for spatially-periodic states of defocussing NLS.

In this paper a bifurcation is identified that gives rise to DSWs. It is the saddle-centre transition of the Floquet multipliers associated with the spatially-periodic states. When considered from the point of view of a (spatial) energy surface, the transition is associated with the coalescence between two spatially periodic states, one of which is spatially elliptic and the other spatially hyperbolic.

The theory will be developed for a general class of Hamiltonian PDEs. The principal requirement is that the steady part is a standard (in general not integrable) Hamiltonian system on \mathbb{R}^4 ,

$$\mathbf{J} \mathbf{u}_x = \nabla S(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^4, \quad (1.4)$$

where \mathbf{J} is the unit symplectic operator

$$\mathbf{J} = \begin{bmatrix} \mathbf{0} & -\mathbf{I} \\ \mathbf{I} & \mathbf{0} \end{bmatrix}, \quad (1.5)$$

and $S(\mathbf{u})$ is the (spatial) Hamiltonian function. The symbol S is used to distinguish it from a temporal Hamiltonian function. Phase space dimension 4 is the lowest dimension that the phenomena occurs. Generalization to higher dimension is possible with appropriate hypotheses on the additional Floquet multipliers (see §6 for discussion). To make it a PDE, add in a time-derivative

term. A large class of Hamiltonian PDEs arise by taking the time-derivative term to be a skew-symmetric matrix times the time derivative

$$\mathbf{M}\mathbf{u}_t + \mathbf{J}\mathbf{u}_x = \nabla S(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^4. \quad (1.6)$$

\mathbf{M} is any constant matrix with $\mathbf{M}^T = -\mathbf{M}$. The skew-symmetry of \mathbf{M} assures that the PDE is conservative. Indeed, this system is an example of a multi-symplectic Hamiltonian PDE (BRIDGES 1997, BRIDGES ET AL. 2010). Here the only property of the time derivative term that will be important is the skew-symmetry of \mathbf{M} . Examples that can be expressed in the form (1.6) are the nonlinear beam equation, NLS, the good Boussinesq equation, and the coupled-mode equation. These examples are discussed in §6 and Appendix D.

The main result of the paper is that the emergence of dark solitary waves is governed by a KdV equation of the following form,

$$\mathcal{A}'(k)q_T + \mathcal{B}''(k)qq_X + \mathcal{K}q_{XXX} = 0, \quad (1.7)$$

for the wavenumber perturbation $q(X, T)$ where X and T are the KdV variables (1.3). This q -KdV equation is on a periodic background. Moreover, the coefficients in the KdV equation are determined by the geometry of the colliding periodic orbits. $\mathcal{A}(k)$ is the *wave action*, $\mathcal{B}(k)$ is the *wave action flux*, and \mathcal{K} is the *Krein signature* of the elliptic periodic orbit in the collision. These geometric properties are developed in §5.

In general Hamiltonian PDEs the emerging waves may be of other related types (e.g. “gray solitary waves”) but for simplicity the term DSW will be used throughout, since the *emergence* has a universal form. DSWs can be stationary or moving at some constant speed, and the periodic state at infinity can be stationary or moving at some speed. For definiteness in this paper, the spatially periodic state is taken to be stationary, and the KdV equation is also constructed relative to an absolute (laboratory) frame of reference.

This theory is to be contrasted with the modulation of spatially-periodic states of reaction-diffusion (RD) equations which requires a time scaling of $T = \varepsilon^2 t$ and leads to a Burgers equation for the perturbation wavenumber q (DOELMAN ET AL. 2009). However, a KdV equation can appear in the RD setting when the wavetrain undergoes modulation instability, and then the modulation equation changes to a KdV equation (VAN HARTEN 1995, DOELMAN ET AL. 2009). The appearance of the KdV equation in the setting of RD equations is more remarkable since the KdV is Hamiltonian and RD equations are in general dissipative. On the other hand, the absence of Hamiltonian structure and conservation of wave action leads to a different form of the KdV equation in the RD setting.

The paper is organized as follows. First the theory of Kivshar is reviewed in §2. Then, with the assumption that there is a branch of periodic states of (1.4), the properties of these states, and the linearization about them is reviewed in §3.

The reduction theory from (1.6) to q -KdV (1.7) is carried out in §4. There are two steps to this theory: expansion in powers of ε and expansion in polynomials of the coordinates of the linearized solution. The theory, particularly conservation of wave action, that leads to the geometric characterization of the coefficients of the KdV equation, is developed in §5. Examples are discussed in §6 and Appendix D. The appendices record details of some of the technical calculations, the definition

of Krein signature, the geometric formulation of the conservation of wave action, and the transformation of the coupled mode equation to the form (1.6).

2. Kivshar's theory for NLS to KdV

In this section the theory of KIVSHAR (1990) is reviewed with emphasis on the case where the basic state is spatially periodic. Take as starting point the following form of the defocussing NLS,

$$iA_t + A_{xx} + A - |A|^2 A = 0. \quad (2.1)$$

The basic class of steady periodic solutions is

$$A(x) = \widehat{A}e^{ikx}, \quad \text{with } \widehat{A} \in \mathbb{R} \quad \text{and} \quad k^2 + \widehat{A}^2 = 1. \quad (2.2)$$

Look for solutions nearby the periodic state of the form

$$A(x, t) = [\widehat{A} + u(x, t)]e^{i(kx + \phi(x, t))}.$$

Substitute into (1.1), separate real and imaginary parts, and introduce the KdV scaling (1.3)

$$\varepsilon^3 u_T + \varepsilon^2 \phi_{XX}(\widehat{A} + u) + 2\varepsilon(k + \varepsilon \phi_X)u_X = 0, \quad (2.3)$$

and

$$\varepsilon^2 u_{XX} - (\widehat{A} + u)[\varepsilon^3 \phi_T + u^2 + 2\widehat{A}u + 2k\varepsilon \phi_X + \varepsilon^2 \phi_X^2] = 0. \quad (2.4)$$

Expand ϕ and u in a power series in ε

$$\phi = \varepsilon \phi_1 + \varepsilon^3 \phi_2 + \dots \quad \text{and} \quad u = \varepsilon^2 u_1 + \varepsilon^4 u_2 + \dots.$$

Substitution then gives the following equations to leading order. For the u -equation (2.3),

$$\begin{aligned} \varepsilon^3: \quad \widehat{A} \frac{\partial^2 \phi_1}{\partial X^2} + 2k \frac{\partial u_1}{\partial X} &= 0 \\ \varepsilon^5: \quad \widehat{A} \frac{\partial^2 \phi_2}{\partial X^2} + 2k \frac{\partial u_2}{\partial X} &= - \left(\frac{\partial u_1}{\partial T} + u_1 \frac{\partial^2 \phi_1}{\partial X^2} + 2 \frac{\partial \phi_1}{\partial X} \frac{\partial u_1}{\partial X} \right), \end{aligned} \quad (2.5)$$

and for the ϕ -equation (2.4),

$$\begin{aligned} \varepsilon^2: \quad (1 - 3\widehat{A}^2 - k^2)u_1 - 2k\widehat{A} \frac{\partial \phi_1}{\partial X} &= 0 \\ \varepsilon^4: \quad (1 - 3\widehat{A}^2 - k^2)u_2 - 2k\widehat{A} \frac{\partial \phi_2}{\partial X} &= \widehat{A} \frac{\partial \phi_1}{\partial T} + 3\widehat{A}u_1^2 - \frac{\partial^2 u_1}{\partial X^2} + 2ku_1 \frac{\partial \phi_1}{\partial X} + \widehat{A} \left(\frac{\partial \phi_1}{\partial X} \right)^2. \end{aligned} \quad (2.6)$$

Differentiate and combine the ε^3 term in (2.5) and the ε^2 term in (2.6),

$$0 = \frac{1}{2k}(1 - 3\widehat{A}^2 + 3k^2) \frac{\partial u_1}{\partial X}$$

For arbitrary u_1 this is satisfied if and only if

$$1 - 3k^2 = 0. \quad (2.7)$$

The significance of this condition will be discussed below. When this condition is satisfied u_1 and ϕ_1 are related by

$$\frac{\partial \phi_1}{\partial X} = -\frac{2k}{\widehat{A}} u_1. \quad (2.8)$$

Now look at the next terms in (2.3) and (2.4), and replace $\frac{\partial \phi_1}{\partial X}$ using (2.8),

$$\widehat{A} \frac{\partial^2 \phi_2}{\partial X^2} + 2k \frac{\partial u_2}{\partial X} = F_1 := -\left(\frac{\partial u_1}{\partial T} - \frac{6k}{\widehat{A}} u_1 \frac{\partial u_1}{\partial X} \right),$$

and

$$(1 - 3\widehat{A}^2 - k^2)u_2 - 2k\widehat{A} \frac{\partial \phi_2}{\partial X} = F_2 := \widehat{A} \frac{\partial \phi_1}{\partial T} + 3\widehat{A}u_1^2 - \frac{\partial^2 u_1}{\partial X^2}.$$

With the condition (2.7), this pair of equations is solvable if and only if

$$\frac{\partial F_2}{\partial X} + 2kF_1 = 0,$$

giving a KdV equation

$$6k^2 \frac{\partial u_1}{\partial T} - \frac{9k}{\widehat{A}} (1 + k^2) u_1 \frac{\partial u_1}{\partial X} + \frac{3}{2} k \frac{\partial^3 u_1}{\partial X^3} = 0.$$

(a) *The Madelung transformation*

Another approach to the reduction from NLS to KdV is to use the *Madelung transformation*. Introduce the transformation $A = \rho(x, t)e^{i\phi}$ in (1.1) and let

$$\rho^2 = \frac{1}{2}gh \quad \text{and} \quad \phi_x = \frac{1}{2}u.$$

Then $h(x, t)$ and $u(x, t)$ satisfy

$$\begin{aligned} h_t + uh_x + hu_x &= 0 \\ u_t + uu_x + gh_x &= \frac{\partial}{\partial x} \left(\frac{h_{xx}}{h} - \frac{1}{2} \frac{h_x^2}{h^2} \right), \end{aligned}$$

which is the shallow water equations with a complicated dispersion term. Near a constant state (h_0, u_0) , this equation can be reduced to a KdV equation when $u_0 = \pm\sqrt{gh_0}$ by uni-directionalization. This approach is used in the rigorous reduction theory of CHIRON & ROUSSET (2010) and BÉTHUEL ET AL. (2009,2010).

(b) *The saddle-centre transition*

In the above derivation of the KdV equation, a necessary condition was (2.7). Let's look more closely at the significance of this condition. The amplitude of the branch of periodic solutions satisfies (2.2), and this curve is shown in Figure 1. The points $(k, \widehat{A}) = \frac{1}{\sqrt{3}}(\pm 1, \sqrt{2})$ are points where the spatial Floquet multipliers go through a hyperbolic-elliptic (saddle-centre) transition. For $-\frac{1}{\sqrt{3}} < k < \frac{1}{\sqrt{3}}$ the branch of periodic solutions is hyperbolic. These features can be verified by direct calculation.

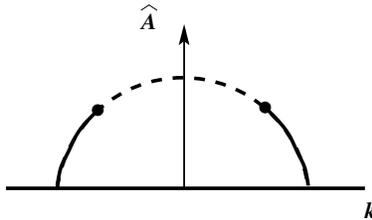


Figure 1. Plot of \hat{A} versus k for the branch of periodic solutions. The change from solid line to dashed line occurs at $(k, \hat{A}) = \frac{1}{\sqrt{3}}(\pm 1, \sqrt{2})$.

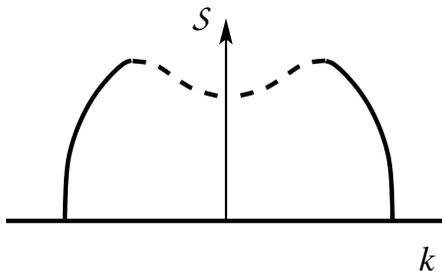


Figure 2. Plot of the spatial energy (2.9) versus wavenumber.

However, the presentation in Figure 1 misses key features of the bifurcation. Consider the “spatial” energy for defocussing NLS,

$$S = \frac{1}{2}|A_x|^2 + \frac{1}{2}|A|^2 - \frac{1}{4}|A|^4,$$

($S_x = 0$ for the steady part of (2.1)) and evaluate on the branch of periodic solutions (2.2)

$$S = \frac{1}{4}(1 - k^2)(1 + 3k^2). \quad (2.9)$$

The spatial energy is plotted in Figure 2. This diagram shows the structure of the bifurcation more clearly. The two maximum points occur at $k = \pm \frac{1}{\sqrt{3}}$ with critical value $S = \frac{1}{3}$. For values of S just below the critical value, there are two periodic solutions with $k > 0$. One is (spatially) elliptic and one (spatially) hyperbolic and as $S \rightarrow \frac{1}{3}$ from below they coalesce, giving birth to the DSW.

On the other hand, it is the wave action flux that will be important in the development of the theory. The wave action flux is defined in §5 and Appendix B, but for purposes of this section it takes the form $\mathcal{B}(k) = k(1 - k^2)$ when evaluated on the branch of periodic states. It is plotted in Figure 3 as a function of wavenumber. In this figure it can be interpreted that as $\mathcal{B}(k)$ approaches its maximum for $k > 0$, an elliptic periodic state collides with a hyperbolic periodic state. These features are general properties of an elliptic-hyperbolic transition of Floquet multipliers along a branch of periodic solutions for a Hamiltonian system on \mathbb{R}^4 , and general aspects of this bifurcation are developed in the next section.

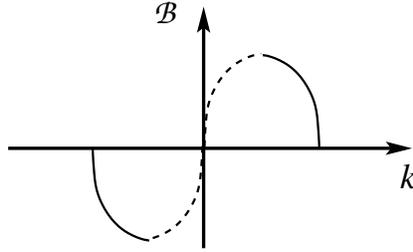


Figure 3. Wave action flux versus wavenumber.

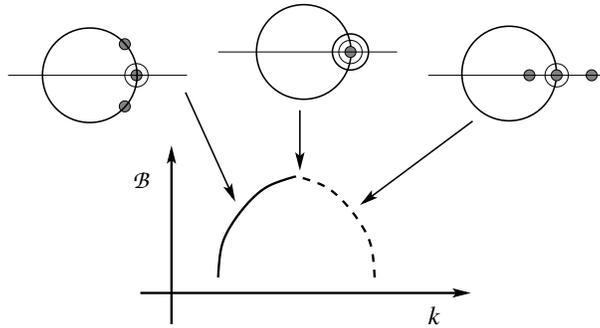


Figure 4. Schematic of the elliptic-hyperbolic transition of Floquet multipliers.

3. Periodic states and the saddle-centre transition

The starting point is the system (1.4). Suppose there exists a one-parameter family of periodic solutions of (1.4),

$$\mathbf{u}(x) := \hat{\mathbf{u}}(\theta, k), \quad \theta = kx + \theta_0, \quad (3.1)$$

where $k > 0$ is the wavenumber of the periodic state, θ_0 is an arbitrary phase shift, and $\hat{\mathbf{u}}$ is a 2π -periodic function of θ . Substituting (3.1) in (1.4) shows that the periodic orbit satisfies

$$k\mathbf{J}\hat{\mathbf{u}}_\theta = \nabla S(\hat{\mathbf{u}}). \quad (3.2)$$

Define the “action” functional by

$$B(\mathbf{u}) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle \mathbf{J}\mathbf{u}_\theta, \mathbf{u} \rangle d\theta. \quad (3.3)$$

Although this functional is the action for the Hamiltonian ODE (1.4) it will be shown later that it is the *wave action flux* associated with the time-dependent Hamiltonian PDE (1.6).

With the definition (3.3), the governing equation (3.2) can be interpreted as the Euler-Lagrange equation for the constrained variational principle: find critical points of the Hamiltonian function restricted to level sets of the action, with k appearing as the Lagrange multiplier. This variational principle is difficult to work

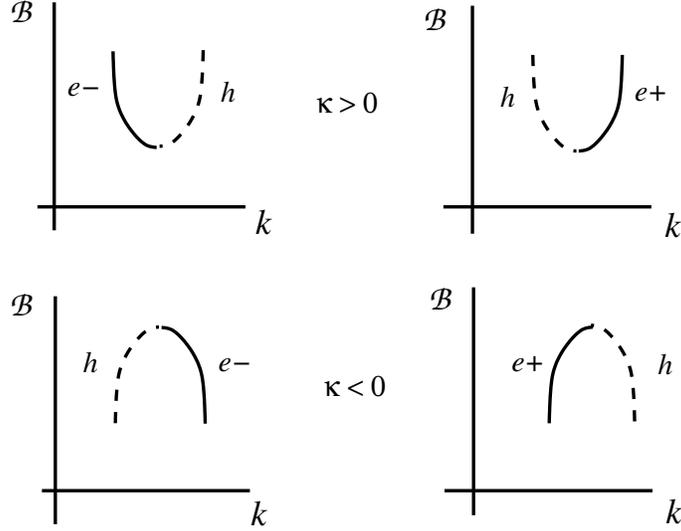


Figure 5. Four cases in the elliptic-hyperbolic transition. h denotes hyperbolic branch of periodic orbits, and $e\pm$ denotes elliptic branch with Krein signature ± 1 .

with since all the critical points have infinite Morse index. On the other hand, the structure from the variational principle will be useful. From the theory of Lagrange multipliers, it follows that a critical point is non-degenerate if $S'(k) \neq 0$ (equivalently $\mathcal{B}'(k) \neq 0$), where

$$S(k) = \frac{1}{2\pi} \int_0^{2\pi} S(\hat{\mathbf{u}}) d\theta \quad \text{and} \quad \mathcal{B}(k) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle \mathbf{J}\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}} \rangle d\theta. \quad (3.4)$$

At points where $S'(k)$ changes sign, a pair of Floquet multipliers coalesces at $+1$. At points where the energy is stationary, the action is also stationary,

$$S'(k) = \langle \nabla S(\hat{\mathbf{u}}), \hat{\mathbf{u}}_k \rangle = k \langle \nabla B(\hat{\mathbf{u}}), \hat{\mathbf{u}}_k \rangle = k\mathcal{B}'(k).$$

Hence $S'(k) = 0$ and $k \neq 0$ imply that $\mathcal{B}'(k) = 0$. Here the double brackets denote the inner product

$$\langle \mathbf{v}, \mathbf{w} \rangle := \frac{1}{2\pi} \int_0^{2\pi} \langle \mathbf{v}(\theta), \mathbf{w}(\theta) \rangle d\theta, \quad (3.5)$$

for any \mathbb{R}^4 -valued 2π -periodic functions $\mathbf{v}(\theta)$ and $\mathbf{w}(\theta)$. The link between Floquet multipliers and $\mathcal{B}(k)$ curves is shown in Figure 4.

There are four cases, and they can each be represented in a (k, \mathcal{B}) diagram as shown in Figure 5. Since $\mathcal{B}'(k) = 0$ at the transition the curves are locally parabolic. Let κ represent the curvature of $\mathcal{B}(k)$ at the transition (a precise definition of κ is given in §4.) In each case an elliptic branch meets a hyperbolic branch and the elliptic branch can have positive or negative Krein signature. The four cases are illustrated in Figure 4. An explicit calculation of the Krein signature, justifying the choices in the figure, is given in Appendix C.

(a) *Linearization at saddle-centre transition*

Now suppose there is a saddle-centre transition of eigenvalues, and look at the linearization of the spatial Hamiltonian system (1.4) about the family of periodic solutions (3.1).

At the transition the algebraic multiplicity of the Floquet multiplier at +1 is (at least) four and the geometric multiplicity is one, but phase space dimension 4 ensures that the algebraic multiplicity equals 4. The Jordan chain theory for this case is given in BRIDGES & DONALDSON (2005).

Firstly, the linearization about a periodic orbit of an autonomous Hamiltonian system always has a Floquet multiplier at +1 of geometric multiplicity one and algebraic multiplicity two. This property follows from differentiation of (3.2) with respect to θ and k ,

$$\mathbf{L}\widehat{\xi}_1(\theta) = 0 \quad \text{and} \quad \mathbf{L}\widehat{\xi}_2(\theta) = \mathbf{J}\widehat{\xi}_1, \quad (3.6)$$

with $\widehat{\xi}_1(\theta) = \widehat{\mathbf{u}}_\theta$, $\widehat{\xi}_2(\theta) = \widehat{\mathbf{u}}_k$ and

$$\mathbf{L} := D^2S(\widehat{\mathbf{u}}(\theta)) - k\mathbf{J}\frac{d}{d\theta}. \quad (3.7)$$

The consequence of the degeneracy $\mathcal{B}'(k) = 0$ is that the algebraic multiplicity of the Floquet multiplier +1 is increased to at least four. In this case, there exists functions

$$\mathbf{L}\widehat{\xi}_3(\theta) = \mathbf{J}\widehat{\xi}_2(\theta) \quad \text{and} \quad \mathbf{L}\widehat{\xi}_4(\theta) = \mathbf{J}\widehat{\xi}_3(\theta).$$

The solutions $\widehat{\xi}_j(\theta)$, $j = 1, 2, 3, 4$ are not unique, and they do not form a symplectic basis with respect to the operator \mathbf{J} . Introduce a normalized basis

$$\begin{aligned} \xi_1(\theta) &= a\widehat{\xi}_1(\theta), & \xi_2(\theta) &= a\widehat{\xi}_2(\theta) \\ \xi_3(\theta) &= a\widehat{\xi}_3(\theta) + b\widehat{\xi}_1(\theta), & \xi_4(\theta) &= a\widehat{\xi}_4(\theta) + b\widehat{\xi}_2(\theta). \end{aligned}$$

where

$$s = \text{sign} \langle \langle \mathbf{J}\widehat{\xi}_4, \widehat{\xi}_1 \rangle \rangle, \quad (3.8)$$

and

$$a = \left| \langle \langle \mathbf{J}\widehat{\xi}_4, \widehat{\xi}_1 \rangle \rangle \right|^{-1/2} \quad \text{and} \quad b = -\frac{1}{2}sa^3 \langle \langle \widehat{\xi}_3, \mathbf{J}\widehat{\xi}_4 \rangle \rangle. \quad (3.9)$$

This set of vectors still forms a Jordan chain:

$$\mathbf{L}\xi_1(\theta) = 0, \quad \mathbf{L}\xi_2(\theta) = \mathbf{J}\xi_1(\theta), \quad \mathbf{L}\xi_3(\theta) = \mathbf{J}\xi_2(\theta), \quad \mathbf{L}\xi_4(\theta) = \mathbf{J}\xi_3(\theta). \quad (3.10)$$

In the transformed basis

$$s = \langle \langle \mathbf{J}\xi_4, \xi_1 \rangle \rangle = \langle \langle \mathbf{J}\xi_2, \xi_3 \rangle \rangle. \quad (3.11)$$

The transformation matrix

$$\Sigma = [\xi_1 \mid \xi_2 \mid -s\xi_4 \mid s\xi_3], \quad (3.12)$$

is symplectic with respect to \mathbf{J} : $\Sigma^T \mathbf{J} \Sigma = \mathbf{J}$. Symplecticity of this transformation is not essential, but it results in the reduced system, leading to q -KdV, having the same spatial symplectic structure as the original system, and it is used in the definition of Krein signature. The purpose of the sign s is to ensure that Σ in (3.12) is symplectic. The sign s is also a symplectic invariant. (Since s is defined

via the symplectic form in (3.11) any symplectic change of coordinates leaves it invariant.)

Taking coordinates (ϕ, q, I, p) the solution of the linear problem in the neighbourhood of the elliptic-hyperbolic transition is

$$\phi\xi_1(\theta) + q\xi_2(\theta) - sI\xi_4(\theta) + sp\xi_3(\theta). \quad (3.13)$$

In the later calculations, equations for the second derivatives of $\hat{\mathbf{u}}(\theta; k)$ will be needed. They are obtained by differentiating the linear equations (3.6),

$$\begin{aligned} \mathbf{L}\hat{\mathbf{u}}_{\theta\theta} &= -D^3S(\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_\theta) \\ \mathbf{L}\hat{\mathbf{u}}_{\theta k} &= -D^3S(\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_k) + \mathbf{J}\hat{\mathbf{u}}_{\theta\theta} \\ \mathbf{L}\hat{\mathbf{u}}_{kk} &= -D^3S(\hat{\mathbf{u}}_k, \hat{\mathbf{u}}_k) + 2\mathbf{J}\hat{\mathbf{u}}_{\theta k}. \end{aligned} \quad (3.14)$$

The formal definition of the third derivative at a point $\hat{\mathbf{u}}$ is

$$\frac{\partial^3}{\partial\epsilon_1\partial\epsilon_2\partial\epsilon_3} \left[\frac{1}{2\pi} \int_0^{2\pi} S(\hat{\mathbf{u}} + \epsilon_1\xi_i + \epsilon_2\xi_j + \epsilon_3\xi_l) d\theta \right] \Big|_{\epsilon=0} = \langle\langle D^3S(\xi_j, \xi_l), \xi_i \rangle\rangle, \quad (3.15)$$

where $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \epsilon_3)$, and the basepoint $\hat{\mathbf{u}}$ is omitted since the context is clear. The right-hand side is invariant under permutation of the three vectors.

4. Scaling, expansion and reduction to KdV

Start with the time-dependent Hamiltonian PDE (1.6) and perturb about the spatially periodic state near a saddle-centre transition,

$$\mathbf{u}(x, t) = \hat{\mathbf{u}}(\theta; k) + \tilde{\mathbf{u}}(\theta, x, t),$$

and substitute into (1.6),

$$\mathbf{M}\tilde{\mathbf{u}}_t + \mathbf{J}\tilde{\mathbf{u}}_x = \nabla S(\hat{\mathbf{u}} + \tilde{\mathbf{u}}) - S(\hat{\mathbf{u}}). \quad (4.1)$$

Drop the tilde on the perturbation, as the context will be clear, and introduce the KdV scaling (1.3),

$$\varepsilon^3 \mathbf{M}\mathbf{u}_T + \varepsilon \mathbf{J}\mathbf{u}_X = \mathbf{L}\mathbf{u} + N(\mathbf{u}), \quad (4.2)$$

where \mathbf{L} is the linear operator from §3, and the nonlinear term is

$$\begin{aligned} N(\mathbf{u}) &= \nabla S(\hat{\mathbf{u}} + \mathbf{u}) - \nabla S(\hat{\mathbf{u}}) - \mathbf{L}\mathbf{u} \\ &= \frac{1}{2}D^3S(\hat{\mathbf{u}})(\mathbf{u}, \mathbf{u}) + \frac{1}{6}D^4S(\hat{\mathbf{u}})(\mathbf{u}, \mathbf{u}, \mathbf{u}) + \dots \end{aligned} \quad (4.3)$$

Henceforth, the derivatives of S will be written without the base point $\hat{\mathbf{u}}$ identified as in (3.15).

The perturbed solution $\mathbf{u}(\theta, X, T, \varepsilon)$, now considered a function of the slow time and space variables instead of x, t , is expanded in a power series in ε . A key

step is to scale the Jordan chain coordinates in (3.13) as

$$\phi \sim \varepsilon, \quad q \sim \varepsilon^2, \quad p \sim \varepsilon^3, \quad I \sim \varepsilon^4. \quad (4.4)$$

Hence the scaled solution for the linear terms is

$$\mathbf{u}^{linear} = \varepsilon\phi(X, T, \varepsilon)\xi_1 + \varepsilon^2q(X, T, \varepsilon)\xi_2 + \varepsilon^3sp(X, T, \varepsilon)\xi_3 - \varepsilon^4sI(X, T, \varepsilon)\xi_4.$$

Now expand the solution \mathbf{u} as a polynomial in the coordinates (ϕ, q, I, p) and with the scaling (4.4),

$$\mathbf{u} = \varepsilon\mathbf{w}_1 + \varepsilon^2\mathbf{w}_2 + \varepsilon^3\mathbf{w}_3 + \varepsilon^4\mathbf{w}_4 + \varepsilon^5\mathbf{w}_5 + \dots, \quad (4.5)$$

with

$$\begin{aligned} \mathbf{w}_1 &= \phi\xi_1 \\ \mathbf{w}_2 &= q\xi_2 + \phi^2\psi_1 \\ \mathbf{w}_3 &= sp\xi_3 + \phi q\psi_2 + \phi^3\chi_1 \\ \mathbf{w}_4 &= -sI\xi_4 + q^2\psi_3 + \phi p\psi_4 + \phi^2q\chi_2 + \phi^4\gamma_1 \\ \mathbf{w}_5 &= qp\psi_5 + \phi I\psi_6 + \phi q^2\chi_3 + \phi^2p\chi_4 + \phi^3q\gamma_2 + \phi^5\gamma_3. \end{aligned}$$

In this expansion the functions ψ_j , $j = 1, \dots, 6$, χ_j , $j = 1, \dots, 4$, and γ_j , $j = 1, 2, 3$ are unknown functions at this point and are used to eliminate terms in the expansion.

Substitute the expansion (4.5) into (4.2) and equate terms proportional to like powers of ε to zero,

$$\begin{aligned} \varepsilon^2 : \quad & (\phi_X - q)\mathbf{J}\xi_1 = \phi^2 A_1^{(2)} + \mathcal{O}_3 \\ \varepsilon^3 : \quad & (q_X - sp)\mathbf{J}\xi_2 = \phi q A_1^{(3)} + \mathcal{O}_3 \\ \varepsilon^4 : \quad & \phi_T \mathbf{M}\xi_1 + s(p_X + I - \frac{1}{2}\kappa q^2)\mathbf{J}\xi_3 = q^2 A_1^{(4)} + \phi p A_2^{(4)} + \mathcal{O}_3 \\ \varepsilon^5 : \quad & q_T \mathbf{M}\xi_2 + 2\phi\phi_T \mathbf{M}\psi_1 - sI_X \mathbf{J}\xi_4 + \phi(p_X + I)\mathbf{J}\psi_4 = qp A_1^{(5)} + \phi I A_2^{(5)} + \mathcal{O}_3, \end{aligned} \quad (4.6)$$

where \mathcal{O}_3 represents terms that are of cubic and higher order in (ϕ, q, I, p) . In the third equation, the term $-\frac{1}{2}s\kappa q^2 \mathbf{J}\xi_3$ is added to the left-hand side with a parameter κ (to be determined) and the same term is added to $A_1^{(4)}$ on the right-hand side. This addition is the natural way to ensure that $A_1^{(4)}$ can be set to zero.

The $A_j^{(m)}$ terms on the right-hand side are

$$\begin{aligned}
A_1^{(2)} &= \mathbf{L}\psi_1 + \frac{1}{2}D^3S(\xi_1, \xi_1) \\
A_1^{(3)} &= \mathbf{L}\psi_2 - 2\mathbf{J}\psi_1 + D^3S(\xi_1, \xi_2) \\
A_1^{(4)} &= \mathbf{L}\psi_3 - \mathbf{J}\psi_2 - \frac{1}{2}s\kappa\mathbf{J}\xi_3 + \frac{1}{2}D^3S(\xi_2, \xi_2) \\
A_2^{(4)} &= \mathbf{L}\psi_4 - s\mathbf{J}\psi_2 + sD^3S(\xi_1, \xi_3) \\
A_1^{(5)} &= \mathbf{L}\psi_5 - 2s\mathbf{J}\psi_3 - \mathbf{J}\psi_4 + sD^3S(\xi_2, \xi_3) \\
A_2^{(5)} &= \mathbf{L}\psi_6 + \mathbf{J}\psi_4 - sD^3S(\xi_1, \xi_4).
\end{aligned} \tag{4.7}$$

The strategy is to show that it is possible to set these six equations to zero, by solving for ψ_j , $j = 1, \dots, 6$. Since \mathbf{L} is symmetric and has a non-trivial kernel, setting each term to zero involves satisfying a solvability condition. Remarkably, all six equations are solvable if and only if

$$\kappa = 3\langle\langle \xi_1, D^3S(\xi_2, \xi_3) \rangle\rangle - 3\langle\langle \xi_1, D^3S(\xi_1, \xi_4) \rangle\rangle - \langle\langle \xi_2, D^3S(\xi_2, \xi_2) \rangle\rangle. \tag{4.8}$$

This expression for κ is important since it will appear later as the coefficient of the nonlinear term in the KdV equation. A proof of this result is in Appendix A.

Set each of the terms in (4.7) to zero in the four equations (4.6), and take the inner product of each equation with ξ_4, \dots, ξ_1 in turn, and use (3.11),

$$\begin{aligned}
\phi_X - q &= \mathcal{O}_3 \\
q_X - sp &= \mathcal{O}_3 \\
\phi_T \langle\langle \mathbf{M}\xi_1, \xi_2 \rangle\rangle - (p_X + I - \frac{1}{2}\kappa q^2) &= \mathcal{O}_3 \\
q_T \langle\langle \mathbf{M}\xi_2, \xi_1 \rangle\rangle + 2\phi\phi_T \langle\langle \mathbf{M}\psi_1, \xi_1 \rangle\rangle - I_X + \phi(p_X + I) \langle\langle \mathbf{J}\psi_4, \xi_1 \rangle\rangle &= \mathcal{O}_3.
\end{aligned}$$

Define

$$m_{12} = \langle\langle \mathbf{M}\xi_1, \xi_2 \rangle\rangle, \quad (\text{and assume that } m_{12} \neq 0). \tag{4.9}$$

The skew-symmetry $\mathbf{M}^T = -\mathbf{M}$ then gives $m_{21} = -m_{12}$. Now, substitute for $(p_X + I)$ from the third equation into the fourth

$$\begin{aligned}
\phi_X - q &= \mathcal{O}_3 \\
q_X - sp &= \mathcal{O}_3 \\
m_{12}\phi_T - (p_X + I - \frac{1}{2}\kappa q^2) &= \mathcal{O}_3 \\
-m_{12}q_T - I_X + (2\langle\langle \mathbf{M}\psi_1, \xi_1 \rangle\rangle + m_{12}\langle\langle \mathbf{J}\psi_4, \xi_1 \rangle\rangle)\phi\phi_T &= \mathcal{O}_3.
\end{aligned} \tag{4.10}$$

The next step is to show that the term proportional to $\phi\phi_T$ can be transformed away. This can be done by introducing a transformation $q = \tilde{q} + b\phi^2$. Substitution

into (4.10) leads to the following equation for b ,

$$0 = 2b\langle\langle\mathbf{M}\xi_2, \xi_1\rangle\rangle + 2\langle\langle\mathbf{M}\psi_1, \xi_1\rangle\rangle + m_{12}\langle\langle\mathbf{J}\psi_4, \xi_1\rangle\rangle.$$

After some simplification, the equation for b reduces to

$$2bm_{12} = a^3\langle\langle\mathbf{M}\hat{\mathbf{u}}_{\theta\theta}, \hat{\mathbf{u}}_{\theta}\rangle\rangle + sm_{12}\langle\langle\xi_4, D^3S(\xi_1, \xi_1)\rangle\rangle.$$

Hence, if $m_{12} \neq 0$ this equation uniquely defines b .

After transformation, neglect of the cubic \mathcal{O}_3 terms, neglect of terms of order ε^6 and higher, and re-ordering of the equations to emphasize the symplectic formulation of the steady part, the reduced equation is

$$\begin{aligned} -m_{12}u_T - I_X &= 0 \\ m_{12}\phi_T - p_X &= I - \frac{1}{2}\kappa q^2 \\ \phi_X &= q \\ q_X &= sp. \end{aligned} \tag{4.11}$$

To see that (4.11) is the KdV equation, differentiate the second equation with respect to X , and eliminate ϕ , I and p reducing it to

$$2m_{12}q_T + \kappa qq_X - sq_{XXX} = 0. \tag{4.12}$$

It remains to show that the coefficients in this KdV equation have a geometric interpretation, and this is done in the next section.

5. Geometry of the coefficients of the KdV equation

In this section the coefficients of the KdV equation (4.12) are given a geometric interpretation. Start with the coefficient of the time-derivative term. From the definition (4.9)

$$m_{12} = \langle\langle\mathbf{M}\xi_1, \xi_2\rangle\rangle = a^2\langle\langle\mathbf{M}\hat{\mathbf{u}}_{\theta}, \hat{\mathbf{u}}_k\rangle\rangle.$$

Using the definition of $\mathcal{A}(k)$ in Appendix B,

$$\mathcal{A}'(k) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle\langle\mathbf{M}\hat{\mathbf{u}}_{\theta k}, \hat{\mathbf{u}}\rangle\rangle d\theta + \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle\langle\mathbf{M}\hat{\mathbf{u}}_{\theta}, \hat{\mathbf{u}}_k\rangle\rangle d\theta = \frac{1}{2\pi} \int_0^{2\pi} \langle\langle\mathbf{M}\hat{\mathbf{u}}_{\theta}, \hat{\mathbf{u}}_k\rangle\rangle d\theta,$$

after integration by parts and using periodicity. But the latter term is $a^{-2}m_{12}$, and so

$$m_{12} = a^2\mathcal{A}'(k). \tag{5.1}$$

To prove that the coefficient κ in (4.11) is proportional to the second derivative of the wave action flux, start with the definition of wave action flux in Appendix

B and differentiate,

$$\mathcal{B}'(k) = \langle\langle \mathbf{J}\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_k \rangle\rangle. \quad (5.2)$$

Taking the second derivative

$$\mathcal{B}''(k) = \langle\langle \mathbf{J}\hat{\mathbf{u}}_{k\theta}, \hat{\mathbf{u}}_k \rangle\rangle + \langle\langle \mathbf{J}\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_{kk} \rangle\rangle. \quad (5.3)$$

The key is to note that $\xi_1 = a\hat{\mathbf{u}}_\theta$ and $\xi_2 = a\hat{\mathbf{u}}_k$ and then use the equations for the second derivatives (3.14). First define

$$\Gamma_i^{jl} = \langle\langle \xi_i, D^3 S(\xi_j, \xi_l) \rangle\rangle, \quad (5.4)$$

and note that it is invariant under permutation of its three indices (cf. (3.15)).

Calculating,

$$\begin{aligned} \mathcal{B}''(k) &= -\frac{1}{a} \langle\langle \mathbf{J}\xi_2, \hat{\mathbf{u}}_{k\theta} \rangle\rangle + \frac{1}{a} \langle\langle \mathbf{J}\xi_1, \hat{\mathbf{u}}_{kk} \rangle\rangle \\ &= -\frac{1}{a} \langle\langle \mathbf{L}\xi_3, \hat{\mathbf{u}}_{k\theta} \rangle\rangle + \frac{1}{a} \langle\langle \mathbf{L}\xi_2, \hat{\mathbf{u}}_{kk} \rangle\rangle \\ &= -\frac{1}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{k\theta} \rangle\rangle + \frac{1}{a} \langle\langle \xi_2, \mathbf{L}\hat{\mathbf{u}}_{kk} \rangle\rangle \\ &= -\frac{1}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{k\theta} \rangle\rangle + \frac{1}{a} \langle\langle \xi_2, -D^3 S(\hat{\mathbf{u}}_k, \hat{\mathbf{u}}_k) + 2\mathbf{J}\hat{\mathbf{u}}_{\theta k} \rangle\rangle \\ &= -\frac{1}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{k\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} - \frac{2}{a} \langle\langle \mathbf{J}\xi_2, \hat{\mathbf{u}}_{\theta k} \rangle\rangle \\ &= -\frac{1}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{k\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} - \frac{2}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{\theta k} \rangle\rangle \\ &= -\frac{3}{a} \langle\langle \xi_3, \mathbf{L}\hat{\mathbf{u}}_{k\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} \\ &= -\frac{3}{a} \langle\langle \xi_3, -D^3 S(\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_k) + \mathbf{J}\hat{\mathbf{u}}_{\theta\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} \\ &= \frac{3}{a^3} \Gamma_3^{12} + \frac{3}{a} \langle\langle \mathbf{J}\xi_3, \hat{\mathbf{u}}_{\theta\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} \\ &= \frac{3}{a^3} \Gamma_3^{12} + \frac{3}{a} \langle\langle \xi_4, \mathbf{L}\hat{\mathbf{u}}_{\theta\theta} \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} \\ &= \frac{3}{a^3} \Gamma_3^{12} - \frac{3}{a} \langle\langle \xi_4, D^3 S(\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}}_\theta) \rangle\rangle - \frac{1}{a^3} \Gamma_2^{22} \\ &= \frac{3}{a^3} \Gamma_3^{12} - \frac{3}{a^3} \Gamma_4^{11} - \frac{1}{a^3} \Gamma_2^{22}, \end{aligned}$$

and so

$$\begin{aligned} a^3 \mathcal{B}''(k) &= 3\Gamma_3^{12} - 3\Gamma_4^{11} - \Gamma_2^{22} \\ &= 3 \langle\langle \xi_3, D^3 S(\xi_1, \xi_2) \rangle\rangle - 3 \langle\langle \xi_4, D^3 S(\xi_1, \xi_1) \rangle\rangle - \langle\langle \xi_2, D^3 S(\xi_2, \xi_2) \rangle\rangle. \end{aligned}$$

Comparison with (4.8) shows that $\kappa = a^3 \mathcal{B}''(k)$. Substitute into (4.12),

$$2a^2 \mathcal{A}'(k) q_T + a^3 \mathcal{B}''(k) q q_X - s q_{XX} = 0.$$

Now use the fact that

$$s = \langle\langle \mathbf{J}\xi_4, \xi_1 \rangle\rangle = a^2 \langle\langle \mathbf{J}\hat{\xi}_4, \hat{\xi}_1 \rangle\rangle,$$

and then a scaling of the form $q = a\tilde{q}$ eliminates a , and a scaling of time eliminates the factor 2, leaving

$$\mathcal{A}'(k) q_T + \mathcal{B}''(k) q q_X + \langle\langle \mathbf{J}\hat{\xi}_1, \hat{\xi}_4 \rangle\rangle q_{XX} = 0.$$

Now a uniform scaling of space and time and setting

$$\mathcal{K} = \text{sign}(\langle\langle \mathbf{J}\widehat{\xi}_1, \widehat{\xi}_4 \rangle\rangle) = -s,$$

then leads to the normal form of the q -KdV equation in (1.7). The connection between Krein signature and the symplectic sign s is given in Appendix C.

This completes the derivation of the q -KdV equation (1.7).

6. Concluding remarks

The assumption of phase space dimension 4 in (1.4) and (1.6) can be relaxed, depending on the position of the other Floquet multipliers. If all the other Floquet multipliers are hyperbolic (even if there are an infinite number) then the theory goes through with a centre-manifold type reduction of the hyperbolic Floquet multipliers. If at least one pair of other Floquet multipliers is elliptic then the theory changes and it is likely that the KdV equation (1.7) will be accompanied by another modulation equation.

No where in the formal construction and reduction to KdV is well-posedness of (1.6) used. Indeed (1.6) can even be elliptic in time. However, for any validity result involving evolution in time well-posedness of (1.6) will be necessary.

The basic spatially-periodic state was assumed stationary relative to an absolute frame of reference. Suppose that it is stationary relative to a frame of reference moving at speed c . Then (1.6) is replaced by

$$\mathbf{M}\mathbf{u}_t + [\mathbf{J} - c\mathbf{M}]\mathbf{u}_x = \nabla S(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^4, \quad (6.1)$$

and then the theory goes through as before with the steady system (1.4) replaced by the c -dependent steady system in (6.1). The moving frame just brings in an additional parameter.

A key structural requirement for the theory is that the PDEs can be formulated as in (1.6). Some examples are (a) the de-focussing NLS equation (1.1), (b) the good Boussinesq equation

$$u_{tt} + u_{xxxx} = (u - u^2)_{xx},$$

and (c) the coupled mode equation (see Appendix D). Details of specific examples will be considered elsewhere.

There are potential applications in the theory of water waves. Unsteady DSWs appear in the theory of water waves when the depth is sufficiently shallow, since the NLS model for water waves is defocussing in that regime (cf. HASIMOTO & ONO 1972, INFELD & ROWLANDS 2000).

However, the theory in this paper suggests that DSWs will emerge at finite amplitude if a saddle-centre transition of eigenvalues occurs in the linearization about travelling waves. Indeed this is the case. VANDENBROECK (1983) computes spatial Floquet multipliers along a branch of Stokes waves and notes the occurrence of a saddle-centre transition. At low amplitude, coupled to a mean flow, BRIDGES & DONALDSON (2006) find saddle-centre transitions analytically. In BRIDGES & DONALDSON (2006) the saddle-centre transition is used as a basis for showing that *steady* DSWs can emerge. The theory in this paper shows that this result can be improved by showing the *unsteady* DSWs can also emerge.

Appendix

Appendix A. Proof that solvability leads to κ

Since \mathbf{L} is formally symmetric, with ξ_1 in the kernel, it follows that

$$\langle\langle \xi_1, \mathbf{L}\psi_j \rangle\rangle = 0, \quad j = 1, \dots, 6. \quad (\text{A-1})$$

Applying this to the six equations in (4.7), results in the two conditions

$$\kappa = 3\langle\langle \xi_1, D^3 S(\xi_2, \xi_3) \rangle\rangle - 3\langle\langle \xi_1, D^3 S(\xi_1, \xi_4) \rangle\rangle - \langle\langle \xi_2, D^3 S(\xi_2, \xi_2) \rangle\rangle. \quad (\text{A-2})$$

and

$$2\langle\langle \xi_1, D^3 S(\xi_1, \xi_3) \rangle\rangle = \langle\langle \xi_1, D^3 S(\xi_2, \xi_2) \rangle\rangle. \quad (\text{A-3})$$

The equation (A-3) is satisfied identically. To verify (A-2) consider solvability of the fifth equation in (4.7), and use the symmetry of \mathbf{L} , (3.10) and the second derivatives (3.14) repeatedly,

$$\begin{aligned} 0 &= \langle\langle \xi_1, \mathbf{L}\psi_5 - 2s\mathbf{J}\psi_3 - \mathbf{J}\psi_4 + sD^3 S(\xi_2, \xi_3) \rangle\rangle \\ &= 2s\langle\langle \mathbf{J}\xi_1, \psi_3 \rangle\rangle + \langle\langle \mathbf{J}\xi_1, \psi_4 \rangle\rangle + s\langle\langle \xi_1, D^3 S(\xi_2, \xi_3) \rangle\rangle \\ &= 2s\langle\langle \mathbf{L}\xi_2, \psi_3 \rangle\rangle + \langle\langle \mathbf{L}\xi_2, \psi_4 \rangle\rangle + s\langle\langle \xi_1, D^3 S(\xi_2, \xi_3) \rangle\rangle \\ &= 2s\langle\langle \xi_2, \mathbf{L}\psi_3 \rangle\rangle + \langle\langle \xi_2, \mathbf{L}\psi_4 \rangle\rangle + s\Gamma_1^{23} \\ &= 2s\langle\langle \xi_2, \mathbf{J}\psi_2 + \frac{1}{2}s\kappa\mathbf{J}\xi_3 - \frac{1}{2}D^3 S(\xi_2, \xi_2) \rangle\rangle + \langle\langle \xi_2, s\mathbf{J}\psi_2 - sD^3 S(\xi_1, \xi_3) \rangle\rangle + s\Gamma_1^{23} \\ &= 3s\langle\langle \xi_2, \mathbf{J}\psi_2 \rangle\rangle + \kappa\langle\langle \xi_2, \mathbf{J}\xi_3 \rangle\rangle - s\langle\langle \xi_2, D^3 S(\xi_2, \xi_2) \rangle\rangle - s\langle\langle \xi_2, D^3 S(\xi_1, \xi_3) \rangle\rangle + s\Gamma_1^{23}. \end{aligned}$$

Noting that the last two terms cancel out, divide by s and use (3.11), then solvability requires

$$\begin{aligned} \kappa &= 3\langle\langle \xi_2, \mathbf{J}\psi_2 \rangle\rangle - \Gamma_2^{22} \\ &= -3\langle\langle \mathbf{J}\xi_2, \psi_2 \rangle\rangle - \Gamma_2^{22} = -3\langle\langle \mathbf{L}\xi_3, \psi_2 \rangle\rangle - \Gamma_2^{22} \\ &= -3\langle\langle \xi_3, \mathbf{L}\psi_2 \rangle\rangle - \Gamma_2^{22} \\ &= -3\Gamma_4^{11} + 3\Gamma_3^{12} - \Gamma_2^{22}, \end{aligned}$$

after repeated use of (3.10) and (3.14). This confirms the expression for κ in (A-2).

Appendix B. Conservation of wave action

Systems of the type (1.6) have a geometrical formulation of conservation of wave action (cf. BRIDGES 1997). Consider an ensemble of solutions $\mathbf{u}(x, t, \theta)$ of (1.6) which is 2π -periodic in the ensemble parameter θ . Define *wave action* and *wave*

action flux as

$$A(\mathbf{u}) = \frac{1}{2} \int_0^{2\pi} \langle \mathbf{M}\mathbf{u}_\theta, \mathbf{u} \rangle d\theta \quad \text{and} \quad B(\mathbf{u}) = \frac{1}{2} \int_0^{2\pi} \langle \mathbf{J}\mathbf{u}_\theta, \mathbf{u} \rangle d\theta. \quad (\text{B-1})$$

Conservation of wave action, $A_t + B_x = 0$, follows from

$$A_t + B_x = - \int_0^{2\pi} \langle \mathbf{M}\mathbf{u}_t + \mathbf{J}\mathbf{u}_x, \mathbf{u}_\theta \rangle d\theta = - \int_0^{2\pi} \langle \nabla S(\mathbf{u}), \mathbf{u}_\theta \rangle d\theta = - \int_0^{2\pi} S_\theta d\theta = 0.$$

Now evaluate the wave action and wave action flux on solutions with $\theta = kx + \theta_0$, and normalize the integrals by 2π ,

$$\mathcal{A}(k) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle \mathbf{M}\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}} \rangle d\theta \quad \text{and} \quad \mathcal{B}(k) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2} \langle \mathbf{J}\hat{\mathbf{u}}_\theta, \hat{\mathbf{u}} \rangle d\theta. \quad (\text{B-2})$$

It is the derivatives with respect to k of these two functions that appear as coefficients in the KdV equation.

Appendix C. Krein signature and the symplectic sign s

In this appendix, the connection between the symplectic sign s and the Krein signature of the elliptic periodic orbit in the collision is established, and the choice of signs $e\pm$ in Figure 4 justified.

The curve of periodic solutions appears in the reduced system as relative equilibrium solutions of (4.11); that is,

$$q = q_0, \quad p = 0, \quad \phi = q_0 x + \phi_0, \quad I = I_0, \quad \text{with} \quad I_0 = \frac{1}{2} \kappa q_0^2,$$

with q_0 and I_0 constants. The (q_0, I_0) curve is a parabola and there are two cases depending on the sign of κ . However, taking into account that there is a change from hyperbolic to elliptic at the maximum (or minimum) of the parabola, there are four cases and they are shown in Figure 5. It remains to establish which branches are elliptic and hyperbolic and the Krein signature of the elliptic branch.

To determine ellipticity or hyperbolicity, only the steady system is required. Linearize the reduced system (4.11) dropping the time derivatives

$$\begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{pmatrix} \phi \\ q \\ I \\ p \end{pmatrix}_X = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -\kappa q_0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & s \end{bmatrix} \begin{pmatrix} \phi \\ q \\ I \\ p \end{pmatrix}. \quad (\text{C-1})$$

Taking solutions proportional to $e^{\mu x}$ results in the characteristic equation

$$0 = \det \begin{bmatrix} 0 & 0 & \mu & 0 \\ 0 & -\kappa q_0 & 1 & \mu \\ -\mu & 1 & 0 & 0 \\ 0 & -\mu & 0 & s \end{bmatrix} = \mu^4 - s\kappa q_0 \mu^2.$$

Hence the nontrivial exponents are

$$\mu^2 = s\kappa q_0,$$

and they are hyperbolic if $s\kappa q_0 > 0$ and elliptic if $s\kappa q_0 < 0$. This confirms the labelling of hyperbolic and elliptic in Figure 5. For Figure 5 q_0 should be interpreted as $k - k_0$, with $\mathcal{B}'(k_0) = 0$, and I_0 should be interpreted at $\mathcal{B}(k) - \mathcal{B}(k_0)$.

Now consider the elliptic case where $-s\kappa q_0 > 0$, and define $\sigma = \sqrt{-s\kappa c}$. The complex eigenvector ζ corresponding to $\mu = i\sigma$ is

$$\zeta = \frac{1}{\sigma^{3/2}} \begin{pmatrix} 1 \\ i\sigma \\ 0 \\ -s\sigma^2 \end{pmatrix}. \quad (\text{C-2})$$

Define the Krein signature, \mathcal{K} , associated with a purely imaginary eigenvalue, with eigenvector ζ , in the linearization about an equilibrium, to be

$$\langle \mathbf{J}\zeta, \bar{\zeta} \rangle = 2i\mathcal{K}. \quad (\text{C-3})$$

The eigenvector ζ in (C-2) has been scaled so that the sign $\mathcal{K} = \pm 1$. Computing the Krein signature for the eigenvalue $i\sigma$ and eigenvector ζ gives

$$2i\mathcal{K} = \langle \mathbf{J}\zeta, \bar{\zeta} \rangle = -2is,$$

and so the Krein sign \mathcal{K} equals $-s$. The resulting Krein signs of each branch are then labelled in Figure 5 as $e\pm$; that is a branch with $e+$ has $\mathcal{K} = +1$ and a branch with $e-$ has $\mathcal{K} = -1$.

Appendix D. Multi-symplectic formulation of the coupled-mode equation

Consider \mathbf{M} in (1.6) to be of the following form

$$\mathbf{M} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}.$$

In this case the operators \mathbf{M} and \mathbf{J} have the interesting properties

$$\mathbf{M}^2 = -\mathbf{I}, \quad \mathbf{J}^2 = -\mathbf{I} \quad \text{and} \quad \mathbf{MJ} = \mathbf{JM}.$$

These properties ensure that the operator $\mathbf{M}\partial_t + \mathbf{J}\partial_x$ is a d'Alembertian operator (symbol of a wave equation).

Taking S to be arbitrary, the system (1.6) has the form

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ v_1 \\ v_2 \end{pmatrix}_t + \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ v_1 \\ v_2 \end{pmatrix}_x = \begin{bmatrix} \partial S / \partial u_1 \\ \partial S / \partial u_2 \\ \partial S / \partial v_1 \\ \partial S / \partial v_2 \end{bmatrix},$$

with coordinates $\mathbf{u} = (u_1, u_2, v_1, v_2)$. A special case of interest is the *coupled mode equation* (GRIMSHAW 2000, GRIMSHAW & CHRISTODOULIDES 2001, GRIMSHAW & SKYRNNIKOV 2002, DERKS & GOTTWALD 2005). To reduce to the coupled

mode equation, take the Hamiltonian function to be

$$\begin{aligned} S(\mathbf{u}) = & \frac{1}{2}\alpha(u_1^2 + u_2^2 - v_1^2 - v_2^2) + \frac{1}{4}a_1(u_1^2 + u_2^2)^2 + \frac{1}{4}a_1(v_1^2 + v_2^2)^2 \\ & + \frac{1}{2}a_2(u_1^2 + u_2^2)(v_1^2 + v_2^2) \\ & + \frac{1}{2}a_3(u_1^2 - u_2^2)(v_1^2 - v_2^2) + 2a_3u_1u_2v_1v_2. \end{aligned}$$

Then with

$$A = u_1 + iu_2 \quad \text{and} \quad B = v_1 + iv_2,$$

the above system can be written in complex form

$$\begin{aligned} -iA_t - B_x - \alpha A &= a_1|A|^2A + a_2|B|^2A + a_3B^2\bar{A} \\ -iB_t + A_x + \alpha B &= a_1|B|^2B + a_2|A|^2B + a_3A^2\bar{B}, \end{aligned}$$

which is the familiar form of the coupled-mode equation. When $a_1 = a_4 = 0$, and parameters are scaled so that $\alpha = a_2 = 1$, the equation reduces to the integrable massive Thirring model (DERKS & GOTTWALD 2005).

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