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Canonical multi-symplectic structure on the total exterior algebra bundle

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The aim of this paper is to construct multi-symplectic structures starting with the geometry of an oriented Riemannian manifold, independent of a Lagrangian or a particular partial differential equation (PDE). The principal observation is that on an n-dimensional orientable manifold M there is a canonical quadratic form $\boldsymbol{\Theta}$ associated with the total exterior algebra bundle on M. On the fibre, which has dimension 2^n, the form $\boldsymbol{\Theta}$ can be locally decomposed into n classical symplectic structures. When concatenated, these n-symplectic structures define a partial differential operator, $\boldsymbol{J}_{\boldsymbol{\partial}}$, which turns out to be a Dirac operator with multi-symplectic structure. The operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ generalizes the product operator $\boldsymbol{J}(\mathrm{d}/\mathrm{d}t)$ in classical symplectic geometry, and M is a generalization of the base manifold (i.e. time) in classical Hamiltonian dynamics. The structure generated by $\boldsymbol{\Theta}$ provides a natural setting for analysing a class of covariant nonlinear gradient elliptic operators. The operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ is elliptic, and the generalization of Hamiltonian systems, $\boldsymbol{J}_{\boldsymbol{\partial}}Z=\nabla S(Z)$, for a section Z of the total exterior algebra bundle, is also an elliptic PDE. The inverse problem—find $S(Z)$ for a given elliptic PDE—is shown to be related to a variant of the Legendre transform on k-forms. The theory is developed for flat base manifolds, but the constructions are coordinate free and generalize to Riemannian manifolds with non-trivial curvature. Some applications and implications of the theory are also discussed.

Keywords: symplecticity; differential forms; nonlinear elliptic PDEs; Dirac operators

1. Introduction

In classical mechanics one can start with a Lagrangian formulation and derive a Hamiltonian formulation by using a Legendre transform. On the other hand, Hamiltonian systems exist independent of a Lagrangian or a differential equation. Given a smooth manifold, there is a natural symplectic structure on the cotangent bundle of the manifold and a vectorfield which preserves the symplectic structure (locally) generates the flow of a Hamiltonian system.

The purpose of this paper is to show that multi-symplectic structures also arise naturally on an oriented Riemannian manifold. Instead of looking on the cotangent bundle, the idea is to look on the total exterior algebra bundle (TEA bundle). However, the organizing centre for this construction is the base manifold rather than the configuration manifold.

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In classical mechanics, the principal manifold is the configuration manifold Q, the manifold of positions, and the cotangent bundle of the configuration manifold T^*Q, the phase space, is a symplectic manifold (cf. ch. 2 of Marsden 1992). In this setting, the geometry of time is absent; time enters only as a way to parameterize paths in the symplectic manifold. Another viewpoint is to make the geometry of time explicit and view position q and its conjugate variable P as local coordinates on the TEA bundle of time; in this case $P = p(t)\mathrm{d}t$, a one form on the time manifold coordinatized by t (this view is elaborated further in §3).

It is the latter view that is the starting point for generalization here. The manifold M is the base manifold: time in classical mechanics, and space or space–time in the PDE setting. The theory will be developed taking the base manifold M to be flat (predominantly $\mathbb{R}^n$ or the flat torus $\mathbb{T}^n := \mathbb{R}^n/\mathbb{Z}^n$), as the motivation is elliptic PDEs arising in symplectic pattern formation. However, the constructions are coordinate free and generalize to Riemannian manifolds with non-trivial curvature.

At each point $x \in M$ considered as an oriented Riemannian manifold with metric[1] $\langle\cdot,\cdot\rangle$, there is an exterior algebra built each of the vector spaces T^*_xM of dimension 2^n denoted by

$$\bigwedge(T^*_xM) = \bigwedge^0(T^*_xM) \oplus \cdots \oplus \bigwedge^n(T^*_xM).$$

The exterior algebra bundle associated with the kth exterior power is constructed by taking a union over M, $\bigwedge^k(T^*M) = \cup_{x\in M}\bigwedge^k(T^*_xM)$. Similarly, the TEA bundle is

$$\bigwedge(T^*M) = \bigcup_{x\in M}\bigwedge^k(T^*_xM).$$

The space of sections of $\bigwedge^k(T^*M)$—differential k-forms—is denoted by $\boldsymbol{\Omega}^k(M)$ (cf. Darling 1994; Rosenberg 1997; Morita 2001). Any $Z \in \boldsymbol{\Omega}(M)$ can be expressed in the form $Z = (\boldsymbol{u}^{(0)}, \boldsymbol{u}^{(1)}, \ldots, \boldsymbol{u}^{(n)})$ with $\boldsymbol{u}^{(k)} \in \boldsymbol{\Omega}^k(M)$.

The starting point of the paper is the observation that there is a canonical quadratic form $\Theta(Z)$ defined on sections of the TEA bundle with values in $\Omega^n(M)$,

$$\Theta(Z) = \sum_{k=1}^{n} \boldsymbol{u}^{(k)} \wedge \star\mathrm{d}\boldsymbol{u}^{(k-1)} = \frac{1}{2}\langle\langle \boldsymbol{J}_{\boldsymbol{\partial}} Z, Z\rangle\rangle \mathrm{d}\mathcal{V} + \mathrm{d}\Upsilon(Z), \tag{1.1}$$

where $\star : \boldsymbol{\Omega}^k(M) \to \boldsymbol{\Omega}^{n-k}(M)$ is the Hodge star operator[2], d_k is the exterior derivative on k-forms, $\mathrm{d}\mathcal{V}$ is a Riemannian volume form, $\langle\langle\cdot,\cdot\rangle\rangle$ is the induced metric on $\bigwedge(T^*M)$,

$$\boldsymbol{J}_{\boldsymbol{\partial}} := \begin{bmatrix} 0 & \delta_1 & 0 & \cdots & 0 & 0 \\ d_0 & 0 & \delta_2 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \ddots & \cdots & 0 \\ 0 & \cdots & 0 & d_{n-2} & 0 & \delta_n \\ 0 & 0 & \cdots & 0 & d_{n-1} & 0 \end{bmatrix}, \tag{1.2}$$

[1] The metric is a positive-definite inner product $\langle\cdot,\cdot\rangle_x$ on T_xM for each $x \in M$, with smooth variation on M. Henceforth, this context will be understood, and the subscript x will be dropped.

[2] The Hodge star operator, $\star := \star_x : \bigwedge^k(T^*_xM) \to \bigwedge^{n-k}(T^*_xM)$ is defined for each $x \in M$ as a pointwise isometry in the usual way (cf. pp. 150–151 of Morita (2001); see §2 for the definition used in this paper), with smooth variation on M.

and $\delta_k{:}\boldsymbol{\Omega}^k(M)\to\boldsymbol{\Omega}^{k-1}(M)$ is the codifferential. (When it is clear which form δ_k or d_k is acting on, the subscript will be dropped.) An explicit expression for the form $\Upsilon(Z)\in\bigwedge(T^*M)$ is given in §2.

The partial differential operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ is a generalization of the operator $\boldsymbol{J}(\mathrm{d}/\mathrm{d}t)$ in classical Hamiltonian dynamics, where

$$\boldsymbol{J}=\begin{pmatrix}0 & -I\\ I & 0\end{pmatrix}.$$

When $n>1$, it is *multi-symplectic* in the following sense: take $M=\mathbb{R}^n$ with coordinates $x=(x_1,\ldots,x_n)$. Then the operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ has the representation

$$\boldsymbol{J}_{\boldsymbol{\partial}}=\boldsymbol{J}_1\frac{\partial}{\partial x_1}+\cdots+\boldsymbol{J}_n\frac{\partial}{\partial x_n}. \tag{1.3}$$

Each of the constant $2^n\times 2^n$ matrices $\boldsymbol{J}_k$, $k=1,\ldots,n$ is skew-symmetric and non-degenerate, and hence they define n-symplectic structures on the vector spaces $\bigwedge(T_x^*M)$. The details of this construction are given in §2 and are based on the following illuminating property of $\boldsymbol{J}_{\boldsymbol{\partial}}$,

$$\boldsymbol{J}_{\boldsymbol{\partial}}\circ\boldsymbol{J}_{\boldsymbol{\partial}}=\mathrm{diag}(\Delta_0,\Delta_1,\ldots,\Delta_n)=-\boldsymbol{I}_N\otimes\Delta, \tag{1.4}$$

where Δ_k is the Laplacian acting on k-forms, Δ is the standard Laplacian on $\mathbb{R}^n$ and $\boldsymbol{I}_N$ is the identity acting on a space of dimension N and in this case $N=2^n$. Equating the right-hand side of (1.4) to the right-hand side of (1.3) composed with itself leads to the identities

$$\boldsymbol{J}_i\boldsymbol{J}_j+\boldsymbol{J}_j\boldsymbol{J}_i=\begin{cases}-2\boldsymbol{I}, & i=j,\\ 0, & i\neq j,\end{cases}\quad i,j=1,\ldots,n. \tag{1.5}$$

Hence the set of symplectic operators $\{\boldsymbol{J}_1,\ldots,\boldsymbol{J}_n\}$ is isomorphic as an associative algebra to the Clifford algebra $\mathcal{C}\ell_{0,n}$ (cf. ch. 14 of Lounesto 1997). The properties (1.4) and (1.5) are reminiscent of the properties of the Dirac operator (cf. Esteban & Séré 2002). The difference here is that the operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ is multi-symplectic and the coefficient matrices each generate a symplectic structure, i.e. the property (1.4) generalizes the property of classical symplectic operators with constant $\boldsymbol{J}:\boldsymbol{J}(\mathrm{d}/\mathrm{d}t)\circ\boldsymbol{J}(\mathrm{d}/\mathrm{d}t)=-\boldsymbol{I}(\mathrm{d}^2/\mathrm{d}t^2)$. One is tempted to call $\boldsymbol{J}_{\boldsymbol{\partial}}$ a 'symplectic Dirac operator', but this term is already used to describe a different class of Dirac operators, based on single-symplectic structure (Habermann 1997). It is named a *multi-symplectic Dirac operator*. Other than the fact that the coefficient matrices generate symplectic structures, the operator has all the usual properties of Dirac operators, and so the functional analytic properties of Dirac operators can be appealed to in the analysis of $\boldsymbol{J}_{\boldsymbol{\partial}}$ (e.g. Gilbert & Murray 1991; Habermann 1997; Roe 1998; Esteban & Séré 2002).

Another interesting property of the operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ is its kernel. Under suitable hypotheses, the kernel of $\boldsymbol{J}_{\boldsymbol{\partial}}$ is the union over k of the harmonic k-forms[3]. Take the simplest non-trivial case for illustration: $M=\mathbb{R}^2$ with $Z=(\phi,\boldsymbol{u},v)\in\boldsymbol{\Omega}^0\oplus\boldsymbol{\Omega}^1\oplus\boldsymbol{\Omega}^2$.

[3] I am grateful to Peter Hydon for this observation.

With $\boldsymbol{u}=u_1\,\mathrm{d}x_1+u_2\,\mathrm{d}x_2$ and $v=v_1\,\mathrm{d}x_1\wedge\mathrm{d}x_2$, setting $\boldsymbol{J}_{\boldsymbol{\partial}}Z=0$ results in

$$\left.\begin{aligned} 0=\delta\boldsymbol{u} &= -\left(\frac{\partial u_1}{\partial x_1}+\frac{\partial u_2}{\partial x_2}\right) && \in\boldsymbol{\Omega}^0(M),\\ 0=\mathrm{d}\phi+\delta v &= \left(\frac{\partial\phi}{\partial x_1}+\frac{\partial v_1}{\partial x_2}\right)\mathrm{d}x_1+\left(\frac{\partial\phi}{\partial x_2}-\frac{\partial v_2}{\partial x_1}\right)\mathrm{d}x_2 && \in\boldsymbol{\Omega}^1(M),\\ 0=\mathrm{d}\boldsymbol{u} &= \left(\frac{\partial u_2}{\partial x_1}-\frac{\partial u_1}{\partial x_2}\right)\mathrm{d}x_1\wedge dx_2 && \in\boldsymbol{\Omega}^2(M),\end{aligned}\right\}\tag{1.6}$$

which is a pair of Cauchy–Riemann equations, with ϕ, v and u_1, u_2 conjugate harmonic functions. Some properties of the kernel of $\boldsymbol{J}_{\boldsymbol{\partial}}$ in n-dimensions are discussed in §2.

This observation generalizes the trivial result in classical symplectic geometry that the kernel of $\boldsymbol{J}(\mathrm{d}/\mathrm{d}t)$ is just the constants (on an appropriate space of functions, such as periodic functions). For example, when $n=1$ and $M=S^1:=\mathbb{R}/\mathbb{Z}$, these constants can be interpreted as the harmonic forms in $\boldsymbol{\Omega}^0(S^1)\oplus\boldsymbol{\Omega}^1(S^1)$! In a more general setting where M is a non-trivial Riemannian manifold with curvature, the kernel of $\boldsymbol{J}_{\boldsymbol{\partial}}$ can be related to the topology of the manifold.

The equation $\boldsymbol{J}_{\boldsymbol{\partial}}Z=0$ is a linear elliptic PDE. By adding an algebraic function of Z to the right-hand side, the equation will still be elliptic, but then it can be nonlinear. Taking a hint from classical Hamiltonian systems, the right-hand side is replaced by the gradient of a functional $S(Z)$,

$$\boldsymbol{J}_{\boldsymbol{\partial}}Z=\nabla S(Z),\quad Z\in\boldsymbol{\Omega}(M).\tag{1.7}$$

At this point, $S:\boldsymbol{\Omega}(M)\to\mathbb{R}$ can be any given smooth functional, subject to the requirement that $\nabla S(Z)$ is in the range[4] of $\boldsymbol{J}_{\boldsymbol{\partial}}$. It is a generalized Hamiltonian functional. The gradient of $S(Z)$ is taken with respect to the induced inner product $\langle\langle\cdot,\cdot\rangle\rangle$. The inverse problem will also be considered: given a class of elliptic PDEs, determine $S(Z)$ so that the PDE has the representation (1.7). A variant of the Legendre transform, which is called a 'Legendre–Hodge transformation', is introduced, with attention restricted to the example $\Delta\phi+V'(\phi)=0$ for illustration, where Δ is the Laplacian, ϕ is scalar-valued and $V(\cdot)$ is a given smooth function.

To see the connection between (1.7) and nonlinear elliptic PDEs, take the example of $M=\mathbb{R}^2$ with the standard Euclidean metric and coordinates (x_1, x_2), and let $Z=(\phi, \boldsymbol{u}, v)\in\boldsymbol{\Omega}(M)$. Then $\boldsymbol{J}_{\boldsymbol{\partial}}Z=\nabla S(Z)$ take the form

$$\left.\begin{aligned}\delta\boldsymbol{u}&=\delta S/\delta\phi,\\ \mathrm{d}\phi+\delta v&=\delta S/\delta\boldsymbol{u},\\ \mathrm{d}\boldsymbol{u}&=\delta S/\delta v.\end{aligned}\right\}\tag{1.8}$$

[4] Either ∇S will be in the range of $\boldsymbol{J}_{\boldsymbol{\partial}}$ by construction or it will be assumed.

Consider the following three examples for $S(Z)$:

$$S(Z)\mathrm{d}\mathcal{V} = \tfrac{1}{2}\,\boldsymbol{u}\wedge\star\boldsymbol{u} + \star\,V(\phi) := (\tfrac{1}{2}[\![\boldsymbol{u},\boldsymbol{u}]\!]_1 + V(\phi))\mathrm{d}\mathcal{V},$$

$$S(Z)\mathrm{d}\mathcal{V} = \tfrac{1}{2}\,\phi\wedge\star\phi + \tfrac{1}{2}\,v\wedge\star v + \star F(\boldsymbol{u}) := (\tfrac{1}{2}[\![\phi,\phi]\!]_0 + \tfrac{1}{2}[\![v,v]\!]_2 + F(\boldsymbol{u}))\mathrm{d}\mathcal{V},$$

$$S(Z)\mathrm{d}\mathcal{V} = \tfrac{1}{2}\,\boldsymbol{u}\wedge\star\boldsymbol{u} + \star H(\phi,v) := (\tfrac{1}{2}[\![\boldsymbol{u},\boldsymbol{u}]\!]_1 + H(\phi,v))\mathrm{d}\mathcal{V}, \tag{1.9}$$

where $V:\boldsymbol{\Omega}^0\to\mathbb{R}$, $F:\boldsymbol{\Omega}^1\to\mathbb{R}$ and $H:\boldsymbol{\Omega}^0\times\boldsymbol{\Omega}^2\to\mathbb{R}$ are given smooth functions, and $[\![\cdot,\cdot]\!]_k$ is the induced inner product on $\bigwedge^k(T^*M)$.

To see the classical form of these PDEs, consider the third example for S in (1.9). Substituting it in (1.8) results in

$$\delta\boldsymbol{u} = H_\phi, \quad \mathrm{d}\phi + \delta v = \boldsymbol{u}, \quad \mathrm{d}\boldsymbol{u} = H_v.$$

Combining these equations results in the coupled semilinear elliptic system of PDEs

$$\delta\mathrm{d}\phi = H_\phi, \quad \mathrm{d}\delta v = H_v, \quad \text{or} \quad \Delta\phi + H_\phi = 0 \quad \text{and} \quad \Delta v + H_v = 0, \tag{1.10}$$

where Δ is the standard Laplacian on $\mathbb{R}^2: \Delta = (\partial^2/\partial x_1^2) + (\partial^2/\partial x_2^2)$. On the other hand, starting with a standard Lagrangian for (1.10) and applying a Legendre transform would not lead to the system (1.8).

The multi-symplectic structure of (1.8) is made explicit by introducing coordinates and using (1.6),

$$\boldsymbol{J}_{\boldsymbol{\partial}}Z = \boldsymbol{J}_1\frac{\partial Z}{\partial x_1} + \boldsymbol{J}_2\frac{\partial Z}{\partial x_2},$$

with

$$\boldsymbol{J}_1 = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{J}_2 = \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}. \tag{1.11}$$

Note that $\boldsymbol{J}_1\boldsymbol{J}_2 + \boldsymbol{J}_2\boldsymbol{J}_1 = 0$, $\boldsymbol{J}_1^2 = -\boldsymbol{I}$ and $\boldsymbol{J}_2^2 = -\boldsymbol{I}$ which are special cases of (1.5). Moreover, the triple of symplectic operators $\{\boldsymbol{J}_1, \boldsymbol{J}_2, \boldsymbol{J}_{12}\}$ generate the quaternions, where $\boldsymbol{J}_{12} = \boldsymbol{J}_1\boldsymbol{J}_2$.

The quadratic form $\boldsymbol{\Theta}$ and the multi-symplectic Dirac operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ generated by it provides the backbone for an intrinsic multi-symplectic formulation for elliptic operators. This theory provides an intrinsic formulation of the multi-symplectic structures in Bridges (1997). There, systems of the form $\sum_{j=1}^n \boldsymbol{J}_j Z_{x_j} = \nabla S(Z)$ are taken as an axiom, and it is shown that such systems are a natural setting for studying existence, bifurcation and stability of symplectic pattern solutions of Hamiltonian PDEs (e.g. Bridges 1998; Bridges & Derks 1999; 2001).

There are many results in the literature on generalizing symplectic geometry to a space–time manifold, going back to the work of Weyl, DeDonder & Cartan in the early part of the twentieth century (cf. Binz *et al.* 1988; Gotay *et al.* 2003 and references therein). The backbone of most of these developments is the *Cartan form* or a generalization of it (e.g. Cantrijn *et al.* 1999).

The Cartan form has advantages and disadvantages. The principal disadvantage is that it relies on the Lagrangian for its geometry, and therefore inherits any problems of the Lagrangian that may be independent of the basic manifolds. The principal advantage is that when it is unique it encodes the geometry of the Lagrangian in an elegant way. See §3 of Gotay (1991) for further discussion of the history and properties of the Cartan form.

An important disadvantage of the Cartan form from the present perspective is that as a model for nonlinear PDEs it leads to equations that are dramatically different from (1.7).

An example will help to see the difference between the multi-symplectic formulation of nonlinear elliptic operators based on $\boldsymbol{\Theta}$ and formulations based on the Cartan form. Consider the following nonlinear PDE on $M=\mathbb{R}^2$:

$$\frac{\partial^2\phi}{\partial x_1^2}+\varepsilon\frac{\partial^2\phi}{\partial x_2^2}+V'(\phi)=0,\quad x=(x_1,x_2)\in M,\quad \varepsilon=\pm 1. \tag{1.12}$$

The elliptic case corresponds to $\varepsilon=+1$ and $\varepsilon=-1$ corresponds to a pseudo-Riemannian metric and leads to a nonlinear wave equation. To construct the Cartan form for this system, the analysis of Marsden & Shkoller (1999) will be followed. They show that the multi-symplectic form (the exterior derivative of the Cartan form) for the system (1.12) is

$$\Omega=\mathrm{d}u\wedge\mathrm{d}\phi\wedge\mathrm{d}x_2-\mathrm{d}v\wedge\mathrm{d}\phi\wedge\mathrm{d}x_1-\mathrm{d}S(Z)\wedge\mathrm{d}x_1\wedge\mathrm{d}x_2,$$

where $Z=(\phi,u,v)\in\mathbb{X}:=\mathbb{R}^3$, $S(Z)=(1/2)u^2+(1/2)\varepsilon v^2+V(\phi)$, and from the Legendre transform: $u=\partial\phi/\partial x_1$ and $v=\varepsilon(\partial\phi/\partial x_2)$. The form Ω is a three form on $M\times\mathbb{X}\cong\mathbb{R}^{2+3}$.

The PDE (1.12) is recovered by requiring $\boldsymbol{i}_{\boldsymbol{X}\Omega}$ to vanish for all vectorfields on $M\times\mathbb{X}$, leading to

$$\boldsymbol{K}_\partial Z=\nabla S(Z),\quad \text{with } \boldsymbol{K}_\partial=\boldsymbol{K}_1\frac{\partial}{\partial x_1}+\boldsymbol{K}_2\frac{\partial}{\partial x_2}, \tag{1.13}$$

where

$$\boldsymbol{K}_1=\begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix}\quad\text{and}\quad \boldsymbol{K}_2=\begin{bmatrix}0&0&-1\\0&0&0\\1&0&0\end{bmatrix}.$$

One can verify that (1.13) is formally equivalent to (1.12), and this equation appears to have a similar form to (1.7) in local coordinates. There is, however, a significant difference that shows up when one attempts to apply analysis to (1.13): *the kernel of $\boldsymbol{K}_\partial$ is in general infinite-dimensional*! The kernel of $\boldsymbol{K}_\partial$ consists of $\{(\phi,u,v)\}$, such that ϕ is constant, $u=\psi_{x_1}$ and $v=-\varepsilon\psi_{x_2}$, with $\psi(x_1,x_2)$ an arbitrary function. Second, the structure operators $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ in (1.13) are lacking any interesting structure other than generating two pre-symplectic structures on $\mathbb{R}^3$, whereas $\boldsymbol{J}_1$, $\boldsymbol{J}_2$, in (1.11) and their product are individually symplectic and generate the quaternions.

The infinite-dimensional kernel can be eliminated by restricting $\boldsymbol{K}_\partial$ to holonomic sections, i.e. consider the operator $\boldsymbol{K}_\partial$ subject to the constraint $u_{x_2}-\varepsilon v_{x_1}=0$. This constraint eliminates the infinite-dimensional kernel, but requires functional analysis with differential constraints which becomes ever more complex as the dimension of the manifold increases. More importantly, however, is that by enlarging the dimension as in (1.8), not only is the functional analysis simplified, but new geometry is revealed.

The problem with the kernel of the left-hand side of (1.13) first arose in the analysis in Bridges & Derks (1999). The problem was eliminated there by adding an additional variable which transformed the matrices $\boldsymbol{K}_1$ and $\boldsymbol{K}_2$ in (1.13) to 4×4 non-degenerate matrices. One of the motivations of the present paper was to determine if there is an intrinsic structure which explains and generalizes the regularization of (1.13) in Bridges & Derks (1999). Indeed, in §4, it is shown that the regularized system of Bridges & Derks can be deduced from the theory of $\boldsymbol{\Theta}$.

The symplectic structures generated by $\boldsymbol{\Theta}$ are also different from the structures in the theory of 'n-symplectic structures' and 'n-symplectic geometry' (e.g. Norris 1993; Lawson 2000; Awane & Goze 2000). Given an n-manifold (not necessarily with a metric), n-symplectic geometry is built on the frame bundle of M using the $\mathbb{R}^n$-valued soldering form. The exterior derivative of the soldering form generates n-symplectic structures on the cotangent bundle of the frame bundle. However, these n-symplectic structures are very different from the n-symplectic structures generated by $\boldsymbol{\Theta}$. In n-symplectic geometry, the individual symplectic structures are degenerate, and hence pre-symplectic, with disjoint kernels, and exist on a manifold of natural dimension $\dim = n + n^2$. The differential equations derived from n-symplectic geometry also have a different structure from those derived from $\boldsymbol{\Theta}$ (Lawson 2000).

An outline of the paper is as follows. In §2, general properties of the form $\boldsymbol{\Theta}$ are presented. In §§3–5, details are presented of the characterization of elliptic operators using the form $\boldsymbol{\Theta}$. The principal example is the nonlinear elliptic PDE $\Delta\phi + V'(\phi) = 0$, and it is shown how a modification of the Legendre transform leads to systems of the form (1.7).

The form $\boldsymbol{\Theta}$ generates PDEs that are covariant. That is, the form of the PDE is invariant under coordinate change. There are many equations in fluid mechanics and pattern formation which are not covariant, but require multi-symplectification. An example is the nonlinear Schrödinger equation (NLS),

$$\mathrm{i}A_t + \Delta A + V'(|A|^2) = 0, \tag{1.14}$$

where $A(x, t)$ is complex-valued, $x \in \mathbb{R}^n$, $V(\cdot)$ is a given smooth function, and Δ is the Laplacian. Time is clearly a preferred direction in this PDE, and so a change of variables which mixed space and time would destroy this preferred direction. For non-covariant PDEs, one uses a hybrid or stratified multi-symplectic structure: the covariant part is generated by $\boldsymbol{\Theta}$, and the time direction generates a symplectic structure on a submanifold of lower dimension. The example of the NLS (1.14) is used in §8 to illustrate this idea of stratification. Detailed examples of the theory will be considered elsewhere.

An intriguing direction is to combine multi-symplectic structures with Morse–Floer theory, by embedding the system (1.7) in a gradient flow. A simple example of this process is applied to multi-symplectic periodic orbits in §7, with speculation about further possibilities in this direction in §7*a*.

2. Properties of $\boldsymbol{\Theta}$

In this section, M is a flat manifold ($\mathbb{R}^n$ or $\mathbb{T}^n := \mathbb{R}^n/\mathbb{Z}^n$) with constant metric based on the standard Euclidean inner product, denoted by $\langle\cdot,\cdot\rangle$. Take local coordinates on M to be $x = (x_1, \ldots, x_n)$, with volume form $\mathrm{d}\mathcal{V} = \mathrm{d}x_1 \wedge \cdots \wedge \mathrm{d}x_n$. This metric induces a metric on T^*M and on each of the bundles $\bigwedge^k(T^*M)$, denoted by $[\![\boldsymbol{u}^{(k)}, \boldsymbol{v}^{(k)}]\!]_k$ for any $\boldsymbol{u}^{(k)}, \boldsymbol{v}^{(k)} \in \boldsymbol{\Omega}^{\mathrm{k}}(M)$. On the TEA bundle $\bigwedge(T^*M)$, the induced metric is denoted by

$$\langle\langle Z, W\rangle\rangle := \sum_{k=0}^{n} [\![\boldsymbol{u}^{(k)}, \boldsymbol{v}^{(k)}]\!]_k, \quad \begin{cases} Z = (\boldsymbol{u}^{(0)}, \dots, \boldsymbol{u}^{(n)}) \in \boldsymbol{\Omega}(M), \\ W = (\boldsymbol{v}^{(0)}, \dots, \boldsymbol{v}^{(n)}) \in \boldsymbol{\Omega}(M). \end{cases} \tag{2.1}$$

The Hodge star operator $\star : \boldsymbol{\Omega}^k(M) \to \boldsymbol{\Omega}^{n-k}(M)$ is normalized by

$$\boldsymbol{u} \wedge \star \boldsymbol{v} = [\![\boldsymbol{u}, \boldsymbol{v}]\!]_k \mathrm{d}\mathcal{V}, \quad \text{for any } \boldsymbol{u}, \boldsymbol{v} \in \boldsymbol{\Omega}^k(M), \tag{2.2}$$

and the codifferential $\delta_{\mathrm{k}} : \boldsymbol{\Omega}^k(M) \to \boldsymbol{\Omega}^{k-1}(M)$ is defined by

$$\delta_k \boldsymbol{u} = (-1)^{nk+n+1} \star d_{n-k} \star \boldsymbol{u}, \quad \text{for any } \boldsymbol{u} \in \boldsymbol{\Omega}^k(M).$$

The following property of $\boldsymbol{J_\partial}$ is due to its definition and the properties of d_k and δ_k.

Proposition 2.1. *Formally, $\boldsymbol{J_\partial}$ maps sections of $\bigwedge(T^*M)$ to sections of $\bigwedge(T^*M)$.*

Remark 2.2. The word 'formally' is used here and throughout the paper to signify that all elements on M will be assumed to be as smooth as required, and the precise (or weakest) smoothness required for each step is not considered.

Proposition 2.3. *Let $Z \in \boldsymbol{\Omega}(M)$ and consider the form $\boldsymbol{\Theta}$ evaluated at Z. Then formally*

$$\boldsymbol{\Theta}(Z) = \frac{1}{2}\langle\langle \boldsymbol{J_\partial} Z, Z\rangle\rangle \mathrm{d}\mathcal{V} + \mathrm{d}\Upsilon(Z), \quad \text{with } \Upsilon(Z) = \frac{1}{2}\sum_{k=1}^{n}\left(\boldsymbol{u}^{(k-1)} \wedge \star \boldsymbol{u}^{(k)}\right) \in \boldsymbol{\Omega}^{n-1}(M).$$

Proof. Using the fact that $\star\star\boldsymbol{u} = (-1)^{k(n-k)}\boldsymbol{u}$ for any $\boldsymbol{u} \in \boldsymbol{\Omega}^k(M)$, and the properties of the codifferential, it follows that $\mathrm{d}\star\boldsymbol{u}^{(k)} = (-1)^k \star \delta \boldsymbol{u}^{(k)}$ and so

$$\begin{aligned}
\boldsymbol{\Theta}(Z) &= \sum_{k=1}^{n} \boldsymbol{u}^{(k)} \wedge \star \mathrm{d}\boldsymbol{u}^{(k-1)} = \frac{1}{2}\sum_{k=1}^{n} \boldsymbol{u}^{(k)} \wedge \star \mathrm{d}\boldsymbol{u}^{(k-1)} + \frac{1}{2}\sum_{k=1}^{n} \mathrm{d}\boldsymbol{u}^{(k-1)} \wedge \star \boldsymbol{u}^{(k)} \\
&= \frac{1}{2}\sum_{k=1}^{n}[\boldsymbol{u}^{(k)} \wedge \star \mathrm{d}\boldsymbol{u}^{(k-1)} + (-1)^k \boldsymbol{u}^{(k-1)} \wedge \mathrm{d}\star\boldsymbol{u}^{(k)}] + \frac{1}{2}\sum_{k=1}^{n}\mathrm{d}(\boldsymbol{u}^{(k-1)} \wedge \star \boldsymbol{u}^{(k)}) \\
&= \frac{1}{2}\sum_{k=1}^{n}[\boldsymbol{u}^{(k)} \wedge \star \mathrm{d}\boldsymbol{u}^{(k-1)} + \boldsymbol{u}^{(k-1)} \wedge \star \delta \boldsymbol{u}^{(k)}] + \mathrm{d}\Upsilon(Z).
\end{aligned}$$

Now use (2.1) and (2.2) and the definition of $\boldsymbol{J_\partial}$,

$$\begin{aligned}
\boldsymbol{\Theta}(Z) &= \frac{1}{2}\sum_{k=1}^{n}[[\![\boldsymbol{u}^{(k)}, \mathrm{d}\boldsymbol{u}^{(k-1)}]\!]_k + [\![\boldsymbol{u}^{(k-1)}, \delta\boldsymbol{u}^{(k)}]\!]_{k-1}]\mathrm{d}\mathcal{V} + \mathrm{d}\Upsilon(Z) \\
&= \frac{1}{2}\left[[\![\boldsymbol{u}^{(0)}, \delta\boldsymbol{u}^{(1)}]\!]_0 + \sum_{k=1}^{n-1}[\![\boldsymbol{u}^{(k)}, \mathrm{d}\boldsymbol{u}^{(k-1)} + \delta\boldsymbol{u}^{(k+1)}]\!]_k + [\![\boldsymbol{u}^{(n)}, \mathrm{d}\boldsymbol{u}^{(n-1)}]\!]_n\right]\mathrm{d}\mathcal{V} + \mathrm{d}\Upsilon(Z) \\
&= \frac{1}{2}\langle\langle \boldsymbol{J_\partial} Z, Z\rangle\rangle \mathrm{d}\mathcal{V} + \mathrm{d}\Upsilon(Z).
\end{aligned}$$

■

Application of Stokes Theorem proves the following.

Corollary 2.4. *Let* $M=\mathbb{T}^n$. *Then*

$$\int_M \Theta(Z) = \int_M \frac{1}{2}\langle\langle \boldsymbol{J}_{\boldsymbol{\partial}} Z, Z\rangle\rangle \mathrm{d}\mathcal{V}.$$

The following result and its corollary are verified by direct calculation.

Proposition 2.5. *For* U, $V\in\boldsymbol{\Omega}(M)$, *with* $U=(\boldsymbol{u}^{(0)}, \dots, \boldsymbol{u}^{(n)})$ *and* $V=(\boldsymbol{v}^{(0)}, \dots, \boldsymbol{v}^{(n)})$,

$$\langle\langle \boldsymbol{J}_{\boldsymbol{\partial}} U, V\rangle\rangle \mathrm{d}\mathcal{V} - \langle\langle U, \boldsymbol{J}_{\boldsymbol{\partial}} V\rangle\rangle \mathrm{d}\mathcal{V} = \mathrm{d}\left(\sum_{j=1}^{n}(\boldsymbol{u}^{(j-1)}\wedge\star\boldsymbol{v}^{(j)} - \boldsymbol{v}^{(j-1)}\wedge\star\boldsymbol{u}^{(j)})\right).$$

Corollary 2.6. *Let* $M=\mathbb{T}^n$. *Then*

$$\int_M \langle\langle \boldsymbol{J}_{\boldsymbol{\partial}} U, V\rangle\rangle \mathrm{d}\mathcal{V} = \int_M \langle\langle U, \boldsymbol{J}_{\boldsymbol{\partial}} V\rangle\rangle \mathrm{d}\mathcal{V},$$

i.e. $\boldsymbol{J}_{\boldsymbol{\partial}}$ *is a symmetric operator with respect to a metric including integration over* M.

One of the most interesting properties of $\boldsymbol{J}_{\boldsymbol{\partial}}$ is its kernel. Define the *Laplace–Beltrami operator* $\Delta_k : \boldsymbol{\Omega}^k(M)\to\boldsymbol{\Omega}^k(M)$ by $\Delta_k := d_{k+1}\delta_k + \delta_{k-1}d_k$. A differential form $\boldsymbol{u}\in\boldsymbol{\Omega}^k(M)$ satisfying $\Delta_k\boldsymbol{u}=0$ is called a harmonic k-form. Denote the harmonic k-forms on M by $\mathcal{H}^k(M)$ and let $\mathcal{H}(M)=\cup_{k=0}^{n}\mathcal{H}^k(M)$.

Proposition 2.7. *With* M *as above, formally,*

$$\boldsymbol{J}_{\boldsymbol{\partial}}\circ\boldsymbol{J}_{\boldsymbol{\partial}} = \mathrm{diag}(\Delta_0, \Delta_1, \dots, \Delta_{n-1}, \Delta_n) = -\boldsymbol{I}_N\otimes\Delta,$$

where $\boldsymbol{I}_N$ *is the identity on* $\mathbb{R}^N$ *with* $N=2^n$, *and* Δ *is the standard Laplacian.*

Proof. The first part follows from the definition of $\boldsymbol{J}_{\boldsymbol{\partial}}$. The second part is proved in Example 4.12 on p. 155 of Morita (2001). ■

Corollary 2.8. *With* M *as above,* $\mathrm{Kernel}(\boldsymbol{J}_{\boldsymbol{\partial}})\subseteq\mathcal{H}(M)$.

Proof. A form $Z\in\Omega(M)\cap\mathcal{H}(\Omega)$ satisfies $\boldsymbol{J}_{\boldsymbol{\partial}}\circ\boldsymbol{J}_{\boldsymbol{\partial}}Z=0$. Hence $\boldsymbol{J}_{\boldsymbol{\partial}}Z=0$ implies $Z\in\mathcal{H}(M)$. ■

The converse, $\mathcal{H}(M)\subseteq\mathrm{Kernel}(\boldsymbol{J}_{\boldsymbol{\partial}})$, will depend on the manifold. Here only the following special case of interest in pattern formation is considered, namely the flat torus with Euclidean metric.

Lemma 2.9. *Suppose* $M=\mathbb{T}^n$. *Then formally* $\mathrm{Kernel}(\boldsymbol{J}_{\boldsymbol{\partial}})=\mathcal{H}(M)$.

Proof. For any smooth $\boldsymbol{u}, \boldsymbol{v}\in\boldsymbol{\Omega}(M)$,

$$\Delta_k\boldsymbol{u}\wedge\star\boldsymbol{u} = \delta\boldsymbol{u}\wedge\star\delta\boldsymbol{u} + \mathrm{d}\boldsymbol{u}\wedge\star\mathrm{d}\boldsymbol{u} + \mathrm{d}[\delta\boldsymbol{u}\wedge\star\boldsymbol{u} - \boldsymbol{u}\wedge\star\mathrm{d}\boldsymbol{u}]. \tag{2.3}$$

When $\boldsymbol{u}\in\boldsymbol{\Omega}(M)$ is harmonic, the left-hand side vanishes. After integration over M, the second term on the right-hand side reduces to an integral over the boundary of $\mathbb{T}^n$, and vanishes due to periodicity. Hence, formally, $\delta_k\boldsymbol{u}=d_k\boldsymbol{u}=0$, for each k, and so $\mathcal{H}(M)\subseteq\mathrm{Kernel}(\boldsymbol{J}_{\boldsymbol{\partial}})$. Combining this result with the corollary of proposition 2.7 completes the proof. ■

Various generalizations, such as Sobolev spaces of functions with assigned boundary values, are also possible (cf. ch. 3 of Schwarz (1995) and references therein for the details of the modifications to Hodge theory), but are not considered here.

Lemma 2.10. *Let M be as above with local coordinates $x=(x_1, \ldots, x_n)$. Then*

$$\boldsymbol{J}_{\boldsymbol{\partial}} = \sum_{j=1}^{n} \boldsymbol{J}_j \frac{\partial}{\partial x_j}, \tag{2.4}$$

and the coefficient matrices $\boldsymbol{J}_j$ satisfy

$$\boldsymbol{J}_i\boldsymbol{J}_j + \boldsymbol{J}_j\boldsymbol{J}_i = 0, \quad i \neq j \quad \text{and} \quad \boldsymbol{J}_i^2 = -\boldsymbol{I}, \quad i = 1, \ldots, n.$$

Proof. The operators 'd' and 'δ' are first-order linear differential operators. Therefore, it is clear that $\boldsymbol{J}_{\boldsymbol{\partial}}$ can be represented as a sum of matrices times ∂_{x_j}.

Substitute (2.4) into the identity in proposition 2.7. For any smooth $Z \in \boldsymbol{\Omega}(M)$, the left-hand side is

$$\boldsymbol{J}_{\boldsymbol{\partial}} \circ \boldsymbol{J}_{\boldsymbol{\partial}} Z = \left(\sum_{i=1}^{n} \boldsymbol{J}_i \partial_{x_i}\right)\left(\sum_{j=1}^{n} \boldsymbol{J}_j \partial_{x_j}\right) Z = \sum_{i=1}^{n}\sum_{j=1}^{n} \boldsymbol{J}_i\boldsymbol{J}_j \frac{\partial^2}{\partial x_i \partial x_j} Z$$

$$= \sum_{j=1}^{n} \boldsymbol{J}_j^2 \frac{\partial^2 Z}{\partial x_j^2} + \sum_{i=1,\ i\neq j}^{n} \sum_{j=1}^{n} \left[\boldsymbol{J}_i\boldsymbol{J}_j + \boldsymbol{J}_j\boldsymbol{J}_i\right] \frac{\partial^2 Z}{\partial x_i \partial x_j}.$$

Equating this expression with $-\boldsymbol{I}_N \otimes \Delta$ leads to the identities. ■

Corollary 2.11. *Each $\boldsymbol{J}_j$ is non-degenerate and skew-symmetric and hence generates a symplectic structure.*

Proof. Skew-symmetry of each $\boldsymbol{J}_j$ follows from the symmetry of $\boldsymbol{J}_{\boldsymbol{\partial}}$ in the corollary of proposition 2.5. Non-degeneracy is immediate from the property $\boldsymbol{J}_i^2 = -\boldsymbol{I}$. ■

One can deduce from the properties of $\boldsymbol{J}_j$ in lemma 2.10 that $\{\boldsymbol{J}_1, \ldots, \boldsymbol{J}_n\}$ generate the Clifford algebra $\mathcal{C}\ell_{(0,n)}$ of the negative definite space $\mathbb{R}^{0,n}$ (Lounesto 1997). The full structure of the Clifford algebra is not inherited because the product in lemma 2.10 is the ordinary matrix product and not a Clifford product. However, this structure does lead to an interesting algebra of symplectic operators. The special cases $n=2$ and 3 are treated in §§4 and 5, respectively.

3. The case $n=1$: classical mechanics from the perspective of the base manifold

In the case $n=1$ with $M=\mathbb{R}$, the form Θ simplifies to $\Theta = P \wedge \star \mathrm{d}q$, where $q \in \boldsymbol{\Omega}^0(M)$ and $P \in \boldsymbol{\Omega}^1(M)$. However, review of this case begins to show how the geometry of the base manifold (in this case time, and so the coordinate will be represented by t) can be used as the organizing centre.

The TEA bundle of time is just the cotangent bundle of time. Take the standard inner product and the standard volume form $\mathrm{d}\mathcal{V} = \mathrm{d}t$. The Hodge star operator has the properties $\star 1 = \mathrm{d}t$ and $\star \mathrm{d}t = 1$, and the codifferential takes the form $\delta_1 \boldsymbol{\omega} = -\star \mathrm{d} \star \boldsymbol{\omega}$ for $\boldsymbol{\omega} \in \boldsymbol{\Omega}^1(M)$.

Classical mechanics for a scalar field, $q: M \to \mathbb{X}$ with $\mathbb{X} = \mathbb{R}$, is a nonlinear elliptic PDE in one dimension,

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} = -V'(q), \tag{3.1}$$

where $V: \mathbb{R} \to \mathbb{R}$ is some given smooth function. Here and throughout, fields will be taken to be scalar-valued (e.g. $q \in \boldsymbol{\Omega}^0(M)$) in order to emphasize the geometry due to the base manifold.

The equation (3.1) is the Euler–Lagrange equation associated with the Lagrangian $\int_{\mathcal{V}} \mathcal{L}$ with Lagrangian density,

$$\mathcal{L} = \tfrac{1}{2}\mathrm{d}q \wedge \star \mathrm{d}q - V(q)\mathrm{d}\mathcal{V}. \tag{3.2}$$

Introduce an effective Legendre transform as follows. Introduce a new variable $P \in \boldsymbol{\Omega}^1(M)$, which in coordinates can be written as $P = p(t)\mathrm{d}t$,

$$\mathcal{L} = \tfrac{1}{2}P \wedge \star P - V(q)\mathrm{d}\mathcal{V} + \alpha \wedge \star(\mathrm{d}q - P), \tag{3.3}$$

where $\alpha \in \boldsymbol{\Omega}^1(M)$ is a Lagrange multiplier. Taking the first variation of $\mathcal{L}$ with respect to P and setting it to zero requires $\alpha = P$, hence $\mathcal{L}$ can be simplified to

$$\mathcal{L} = P \wedge \star \mathrm{d}q - \tfrac{1}{2}P \wedge \star P - V(q)\mathrm{d}\mathcal{V}. \tag{3.4}$$

This Lagrangian is the density for *Hamilton's principle* (cf. Weinstein 1978)—viewed from the base manifold: $p\,\mathrm{d}q$ on T^*Q is replaced by $P \wedge \star \mathrm{d}q$ on M.

Now, take the first variation of the Lagrangian (3.4),

$$\left.\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{L}(q+\epsilon\hat{q}, P)|_{\epsilon=0} &= -V'(q)\hat{q}\,\mathrm{d}t + \mathrm{d}\hat{q} \wedge \star P \\ &= -V'(q)\hat{q}\,\mathrm{d}t - \hat{q} \wedge \mathrm{d}\star P + \mathrm{d}(\hat{q} \wedge \star P), \\ \frac{\mathrm{d}}{\mathrm{d}\epsilon}\mathcal{L}(q, P+\epsilon\hat{P})|_{\epsilon=0} &= -\hat{P} \wedge \star P + \hat{P} \wedge \star \mathrm{d}q. \end{aligned}\right\}$$

Integrating and taking vanishing endpoint conditions leads to

$$\left.\begin{aligned} \delta P &= V'(q), \quad \text{in } \boldsymbol{\Omega}^0(M), \\ \mathrm{d}q &= P, \quad \text{in } \boldsymbol{\Omega}^1(M), \end{aligned}\right\} \quad \text{or} \quad \begin{bmatrix} 0 & \delta_1 \\ d_0 & 0 \end{bmatrix} \begin{pmatrix} q \\ P \end{pmatrix} = \begin{pmatrix} V'(q) \\ P \end{pmatrix}, \tag{3.5}$$

equivalently, $\boldsymbol{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$ when $S = \star((1/2)P \wedge \star P) + V(q)$. In coordinates this equation takes the familiar form

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} q \\ p \end{pmatrix}_t = \begin{pmatrix} V'(q) \\ p \end{pmatrix}.$$

However, it is the coordinate-free representation (3.5)—coordinate free on the base manifold—which generalizes most easily to the case where the dimension of M is greater than 1.

4. The case n=2: towards a Legendre–Hodge transformation

Let $M=\mathbb{R}^2$ with coordinates $x=(x_1, x_2)$ and volume form $\mathrm{d}\mathcal{V}=\mathrm{d}x_1\wedge \mathrm{d}x_2$. For the metric, take the standard Euclidean inner product denoted by $\langle\cdot,\cdot\rangle$. The TEA at each point has dimension 4. Let $Z=(\phi, \boldsymbol{u}, v)$ represent an arbitrary element in $\boldsymbol{\Omega}(M)$. Then

$$\Theta(Z) = \boldsymbol{u}\wedge \star\mathrm{d}\phi + v\wedge \star\mathrm{d}\boldsymbol{u},$$

where the action of Hodge star is $\star\mathrm{d}x_1=\mathrm{d}x_2$, $\star\mathrm{d}x_2=-\mathrm{d}x_1$ and $\star 1=\mathrm{d}\mathcal{V}$, with codifferential $\delta\boldsymbol{u}=-\star\mathrm{d}\star\boldsymbol{u}$, $u\in\boldsymbol{\Omega}^j(M)$, $j=1, 2$.

Consider the following generalization of (3.1),

$$\frac{\partial^2\phi}{\partial x_1^2}+\frac{\partial^2\phi}{\partial x_2^2} = -V'(\phi), \tag{4.1}$$

where $\phi: M\to\mathbb{X}$, with $\mathbb{X}=\mathbb{R}$ (e.g. $\phi\in\boldsymbol{\Omega}^0(M)$ and V is a given smooth function. The standard Lagrangian density for (4.1) is (3.2) with appropriate modification for the change of M. Apply an effective Legendre transform by introducing a new variable $\boldsymbol{u}\in\boldsymbol{\Omega}^1(M)$. Enforcing this constraint is a Lagrange multiplier $\boldsymbol{\alpha}\in\boldsymbol{\Omega}^1(M)$,

$$\mathcal{L} = \tfrac{1}{2}\boldsymbol{u}\wedge\star\boldsymbol{u} - V(\phi)\mathrm{d}\mathcal{V} + \boldsymbol{\alpha}\wedge\star(\mathrm{d}\phi-\boldsymbol{u}) + v\wedge\star\mathrm{d}\boldsymbol{\alpha}. \tag{4.2}$$

However, the form $\boldsymbol{\alpha}$ is not a general form in $\boldsymbol{\Omega}^1(M)$: it is required to be a closed form. Therefore, $\mathrm{d}\boldsymbol{\alpha}=0$ is added as a constraint which in turn generates a further Lagrange multiplier $v\in\boldsymbol{\Omega}^2(M)$.

No further constraint is needed as v is proportional to the volume form. The standard Legendre transform would have $\boldsymbol{\alpha}=v=0$. This modified Legendre transform is called a Legendre–Hodge transform, because the new forms are suggested by the Hodge decomposition of each Lagrange multiplier.

As in the one-dimensional case, the variation with respect to $\boldsymbol{u}$ results in $\boldsymbol{\alpha}=\boldsymbol{u}$, and (4.2) can immediately be simplified to

$$\mathcal{L} = -\tfrac{1}{2}\boldsymbol{u}\wedge\star\boldsymbol{u} - V(\phi)\mathrm{d}\mathcal{V} + \boldsymbol{u}\wedge\star\mathrm{d}\phi + v\wedge\star\mathrm{d}\boldsymbol{u} = \Theta(Z) - S(\phi,\boldsymbol{u})\mathrm{d}\mathcal{V}, \tag{4.3}$$

with $S(\phi,\boldsymbol{u})=(1/2)[\![\boldsymbol{u},\boldsymbol{u}]\!]_1+V(\phi)$. This Lagrangian density is a generalization of the density for Hamilton's principle—viewed from the base manifold.

Now take the first variation of the Lagrangian (4.3),

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{L}(\phi+\varepsilon\hat{\phi},\boldsymbol{u},v)|_{\varepsilon=0} = -V'(\phi)\hat{\phi}\,\mathrm{d}\mathcal{V} - \hat{\phi}\wedge\mathrm{d}\star\boldsymbol{u} + \mathrm{d}(\hat{\phi}\wedge\star\boldsymbol{u}),$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{L}(\phi,\boldsymbol{u}+\varepsilon\hat{\boldsymbol{u}},v)|_{\varepsilon=0} = -\hat{u}\wedge\star\boldsymbol{u} + \hat{\boldsymbol{u}}\wedge\star\mathrm{d}\phi + \hat{u}\wedge\mathrm{d}\star v + \mathrm{d}(\hat{\boldsymbol{u}}\wedge\star v),$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathcal{L}(\phi,\boldsymbol{u},v+\varepsilon\hat{v},)|_{\varepsilon=0} = \hat{v}\wedge\star\mathrm{d}\boldsymbol{u}.$$

Integrating and taking the variations $(\hat{\phi},\hat{\boldsymbol{u}},\hat{v})$ to vanish at the boundary leads to (after acting on each equation with Hodge star)

$$\left.\begin{aligned} \delta\boldsymbol{u} &= V'(\phi), && \text{in } \boldsymbol{\Omega}^0(M),\\ \mathrm{d}\phi+\delta v &= \boldsymbol{u}, && \text{in } \boldsymbol{\Omega}^1(M),\\ \mathrm{d}\boldsymbol{u} &= 0, && \text{in } \boldsymbol{\Omega}^2(M), \end{aligned}\right\} \tag{4.4}$$

or $\boldsymbol{J}_{\boldsymbol{\partial}} Z = \nabla S(Z)$. Introducing standard coordinates, $\boldsymbol{u} = u_1\,\mathrm{d}x_1 + u_2\,\mathrm{d}x_2$ and $v = v_1\,\mathrm{d}\mathcal{V}$,

$$\boldsymbol{u}\wedge\star\mathrm{d}\phi = \left(u_1\frac{\partial\phi}{\partial x_1} + u_2\frac{\partial\phi}{\partial x_2}\right)\mathrm{d}x_1\wedge\mathrm{d}x_2,$$

$$v\wedge\star\mathrm{d}\boldsymbol{u} = v\left(\frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}\right) = v_1\left(\frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}\right)\mathrm{d}x_1\wedge\mathrm{d}x_2,$$

leading to $\boldsymbol{J}_1(\partial Z/\partial x_1) + \boldsymbol{J}_2(\partial Z/\partial x_2) = \nabla S(Z)$, where $\boldsymbol{J}_1$ and $\boldsymbol{J}_2$ are defined in (1.11).

5. The operator $\boldsymbol{J}_{\boldsymbol{\partial}}$ when $M = \mathbb{R}^3$

Let $M = \mathbb{R}^3$ with coordinates $x = (x_1, x_2, x_3)$ and volume form $\mathrm{d}\mathcal{V} = \mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3$. The TEA built on T_x^*M has dimension 8. The purpose of this section is twofold. It illustrates the case where two additional constraints are required, and gives coordinate results for $\boldsymbol{J}_{\boldsymbol{\partial}}$ which are of interest in applications. Since the constructions are similar to §§3 and 4, just a sketch is given, highlighting the new features.

Consider the semilinear elliptic PDE $\Delta\phi + V'(\phi) = 0$. The standard Lagrangian density is the same as (3.2) extended to $M = \mathbb{R}^3$. Adding constraints,

$$\mathcal{L} = \tfrac{1}{2}\boldsymbol{u}\wedge\star\boldsymbol{u} - V(\phi)\mathrm{d}\mathcal{V} + \boldsymbol{\alpha}\wedge\star(\mathrm{d}\phi - \boldsymbol{u}) + \boldsymbol{v}\wedge\star\mathrm{d}\boldsymbol{\alpha} + w\wedge\star\mathrm{d}\boldsymbol{v}, \qquad (5.1)$$

where $\boldsymbol{\alpha}\in\boldsymbol{\Omega}^1(M)$, $\boldsymbol{v}\in\boldsymbol{\Omega}^2(M)$ and $w\in\boldsymbol{\Omega}^3(M)$ are Lagrange multipliers. Simplifying,

$$\mathcal{L} = -S(\phi,\boldsymbol{u})\mathrm{d}\mathcal{V} + \boldsymbol{u}\wedge\star\mathrm{d}\phi + \mathrm{v}\wedge\star\mathrm{d}\boldsymbol{u} + w\wedge\star\mathrm{dv} = \Theta(Z) - S(\phi,\boldsymbol{u})\mathrm{d}\mathcal{V}, \qquad (5.2)$$

with $S(\phi,\boldsymbol{u}) = (1/2)[\![\boldsymbol{u},\boldsymbol{u}]\!]_1 + V(\phi)$ and $Z = (\phi, \boldsymbol{u}, \boldsymbol{v}, w)\in\boldsymbol{\Omega}(M)$.

Taking the first variation of the Lagrangian (5.2) and acting on each equation with Hodge star leads to

$$\delta\boldsymbol{u} = V'(\phi), \quad \mathrm{d}\phi + \delta\boldsymbol{v} = \boldsymbol{u}, \quad \mathrm{d}\boldsymbol{u} + \delta w = 0, \quad \mathrm{d}\boldsymbol{v} = 0, \qquad (5.3)$$

which is in the standard form $\boldsymbol{J}_{\boldsymbol{\partial}}Z = \nabla S(Z)$. In coordinates,

$$\begin{aligned}\boldsymbol{u} &= u_1\,\mathrm{d}x_1 + u_2\,\mathrm{d}x_2 + u_3\,\mathrm{d}x_3,\\ \boldsymbol{v} &= v_1\,\mathrm{d}x_2\wedge\mathrm{d}x_3 + v_2\,\mathrm{d}x_3\wedge\mathrm{d}x_1 + v_3\,\mathrm{d}x_1\wedge\mathrm{d}x_2,\\ \boldsymbol{w} &= w_1\,\mathrm{d}x_1\wedge\mathrm{d}x_2\wedge\mathrm{d}x_3;\end{aligned}$$

and so, the system (5.3) takes the form,

$$\boldsymbol{J}_1\frac{\partial Z}{\partial x_1} + \boldsymbol{J}_2\frac{\partial Z}{\partial x_2} + \boldsymbol{J}_3\frac{\partial Z}{\partial x_3} = \nabla S(Z), \quad Z\in\boldsymbol{\Omega}(M),$$

with

$$J_1 = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}, \quad J_2 = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

and

$$J_3 = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad Z = \begin{pmatrix} \phi \\ u_1 \\ u_2 \\ u_3 \\ v_1 \\ v_2 \\ v_3 \\ w_1 \end{pmatrix}.$$

It follows from lemma 2.10 that the symplectic operators $\{\boldsymbol{J}_1, \boldsymbol{J}_2, \boldsymbol{J}_3\}$ satisfy

$$\boldsymbol{J}_1^2 = \boldsymbol{J}_2^2 = \boldsymbol{J}_3^2 = -\boldsymbol{I} \quad \text{and} \quad \boldsymbol{J}_1\boldsymbol{J}_2 + \boldsymbol{J}_2\boldsymbol{J}_1 = \boldsymbol{J}_1\boldsymbol{J}_3 + \boldsymbol{J}_3\boldsymbol{J}_1 = \boldsymbol{J}_2\boldsymbol{J}_3 + \boldsymbol{J}_3\boldsymbol{J}_2 = 0.$$

The set of double products $\{\boldsymbol{J}_{12}, \boldsymbol{J}_{13}, \boldsymbol{J}_{23}\}$, where $\boldsymbol{J}_{ij} := \boldsymbol{J}_i\boldsymbol{J}_j$ also consists of symplectic operators, and they generate the quaternions. The triple product $\boldsymbol{J}_1\boldsymbol{J}_2\boldsymbol{J}_3$ is an involution.

The theory carries over in a straightforward way to the class of elliptic PDES $\delta \mathrm{d}\phi = V'(\phi)$ on $M = \mathbb{R}^n$, with $n > 3$.

6. Periodic patterns and the loop space

In symplectic pattern formation, the existence, bifurcation and stability of multi-periodic patterns of gradient elliptic PDEs is of interest (Bridges 1998). In this section, one of the properties of the PDEs generated by $\boldsymbol{\Theta}$ on periodic patterns is illustrated.

Consider the multi-symplectic PDE (1.7) with $M = \mathbb{T}^n$ in local coordinates,

$$\sum_{j=1}^{n} \boldsymbol{J}_j \frac{\partial Z}{\partial x_j} = \nabla S(Z), \quad Z \in \boldsymbol{\Omega}(M). \tag{6.1}$$

In the case $n=1$, it reduces to the case of periodic solutions of a classical Hamiltonian ODE which can be characterized as relative equilibria on the loop space of the symplectic manifold (cf. Weinstein 1978).

When $n=1$ and $S(Z)$ in (6.1) does not depend explicitly on M (autonomous), every *non-degenerate* periodic solution[5] has a $\mathbb{Z}_2$-valued function associated with it: the sign of the frequency map, $\omega'(I)$, where I is the value of the level set of the action evaluated on the periodic orbit. Equivalently, the sign of $T'(h)$, where T is the period and h the value of the Hamiltonian level set (Bates & Śniatycki 1992).

This $\mathbb{Z}_2$ invariant can be generalized to multi-symplectic PDEs by generalizing Weinstein's characterization of periodic orbits. There are a number of ways to generalize to systems of the form $\boldsymbol{J}_{\boldsymbol{\partial}}Z=\nabla S(Z)$ and the simplest such generalization will be given here.

Since M is flat, let $\mathbb{V}=\bigwedge(T_x^*M)$ and identify the vector spaces for all $x\in\mathbb{M}$. The dimension of $\mathbb{V}$ is 2^n and it can be identified with $\mathbb{R}^{2^n}$ with the induced metric. Now, consider (6.1) restricted to loops, i.e. mappings of the form

$$\hat{Z}(\theta):\mathbb{S}^1\rightarrow\mathbb{V},\quad \text{with } \theta=\boldsymbol{\omega}\cdot x+\theta_0, \tag{6.2}$$

where $\boldsymbol{\omega}=(\omega_1,\ldots,\omega_n)$ and θ_0 is an arbitrary phase shift. Substitution into (6.1) results in

$$\sum_{j=1}^{n}\omega_j\boldsymbol{J}_j\frac{\mathrm{d}\hat{Z}}{\mathrm{d}\theta}=\nabla S(\hat{Z}). \tag{6.3}$$

Define

$$\mathcal{A}_j(Z)=\oint\tfrac{1}{2}\langle\langle\boldsymbol{J}_jZ_\theta,Z\rangle\rangle\mathrm{d}\theta,\quad j=1,\ldots,n.$$

Then solutions of the form (6.2) can be formally characterized as critical points of $\oint S(Z)\mathrm{d}\theta$ restricted to level sets of the n functionals $\mathcal{A}_j(Z)$, in which case the ω_j are Lagrange multipliers. This constrained variational principle is said to be non-degenerate when

$$\det\left[\frac{\delta\boldsymbol{\omega}}{\delta I}\right]\neq0,\quad \text{where } \frac{\delta\boldsymbol{\omega}}{\delta I}=\begin{bmatrix}\dfrac{\partial\omega_1}{\partial I_1} & \cdots & \dfrac{\partial\omega_1}{\partial I_n}\\ \vdots & \ddots & \vdots\\ \dfrac{\partial\omega_n}{\partial I_1} & \cdots & \dfrac{\partial\omega_n}{\partial I_n}\end{bmatrix}, \tag{6.4}$$

where $I=(I_1,\ldots,I_n)$ and I_j is the value of the level set of $\mathcal{A}_j$.

This variational principle is highly indefinite and so it would be difficult to apply direct methods of the calculus of variations. However, a range of variational principles of this type arise in symplectic pattern formation (Bridges 1997, 1998), and some useful information can be extracted. One of the intriguing features of the present coordinate-free formulation is that a generalization of Morse–Floer theory is conceivable. Some results towards this are presented in §7 based on the above variational principle.

[5] See Bridges & Donaldson (2005) for recent results on the universal behaviour near *degenerate* periodic orbits.

7. Multi-symplectic periodic orbits and the gradient flow

Application of Morse theory to periodic solutions of Hamiltonian systems is notoriously difficult, because the functional associated with Hamilton's principle on the loop space is highly indefinite (Abbondandolo 2001), and this difficulty has led to the development of the theory of Floer (1988). In this section, it is shown how multi-symplectic systems can be embedded in a gradient flow and a hint of the type of result one can obtain is given.

Consider the multi-symplectic PDE (1.7) embedded in a gradient flow in the time direction,

$$Z_t + \boldsymbol{J}_{\boldsymbol{\partial}} Z = \nabla S(Z), \tag{7.1}$$

in the neighbourhood of a periodic orbit $\hat{Z}(\theta)$ satisfying (6.3). In Morse theory or Floer theory, one is interested in the manifold of orbits of (7.1) which connect different solutions of (6.3). Here, the analysis of the linearization will be given, which provides information on the stable and unstable subspaces in the gradient flow.

In addition to the fact that the system is multi-symplectic, there are two other aspects of the approach here that are non-standard. First, the loop is taken to be a solution of the 'autonomous' system, i.e. S is independent of x. The reason for this is that the frequency map plays an important role in the autonomous case. Second, the perturbed problem will be studied on a space of functions which is larger than the obvious one. Effectively, functions on the universal cover of $\mathbb{S}^1$ will be considered rather than functions on $\mathbb{S}^1$.

Let $\hat{Z}(\theta)$ be a solution of (6.3) that is continuously differentiable in both θ and ω, and non-degenerate (satisfies (6.4)). Such solutions can be shown to exist for a wide range of Hamiltonian functions $S(Z)$, since (6.3) is a reduction to an ODE of the multi-symplectic PDE. Take $Z(x,t) = \hat{Z}(\theta) + \hat{U}(\theta,x,t)$, substitute into (7.1) and linearize about $\hat{Z}(\theta)$,

$$\hat{U}_t + \boldsymbol{J}_1 \hat{U}_{x_1} + \cdots + \boldsymbol{J}_n \hat{U}_{x_n} = \boldsymbol{L}\hat{U}, \tag{7.2}$$

where

$$\boldsymbol{L}\hat{U} := D^2 S(\hat{Z})\hat{U} - \sum_{j=1}^{n} \omega_j \boldsymbol{J}_j \hat{U}_\theta = D^2 S(\hat{Z})\hat{U} - \sum_{j=1}^{n} \omega_j D^2 \mathcal{A}_j(\hat{Z})\hat{U}.$$

Take the spectral ansatz $\hat{U}(\theta,x,t) = \mathrm{e}^{\lambda t} U(\theta,x)$, and since the coefficients of $\boldsymbol{L}$ do not depend on x, take a Fourier transform in x. Then the analysis of (7.1) near a loop reduces the analysis of the parameter-dependent spectral problem

$$\boldsymbol{L}U = \lambda U + \sum_{j=1}^{n} \mathrm{i}\alpha_j \boldsymbol{J}_j U, \quad U \in \mathbb{V}^{\mathbb{C}}, \tag{7.3}$$

where $\mathbb{V}^{\mathbb{C}}$ is the complexification of the vector space $\mathbb{V}$ introduced in §6, and $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)$ is the Fourier transform parameter, taken to be real.

The natural space to study this spectral problem is $\boldsymbol{L}^2(\mathbb{S}^1, \mathbb{V}^{\mathbb{C}})$. In this space, $\boldsymbol{L}$ is well defined as a mapping from $\mathcal{D}(\boldsymbol{L}) \to L^2(\mathbb{S}^1, \mathbb{V}^{\mathbb{C}})$ and the domain of $\boldsymbol{L}$, $\mathcal{D}(\boldsymbol{L})$, can be taken to the Hilbert space $H^1(\mathbb{S}^1, \mathbb{V}^{\mathbb{C}})$.

With the assumed smoothness of $\hat{Z}$, the governing equation for $\hat{Z}$ can be differentiated with respect to θ to confirm that

$$\mathrm{span}\{\hat{Z}_\theta\} \subseteq \mathrm{Kernel}(\boldsymbol{L}). \tag{7.4}$$

The linearization of the gradient flow has a neutral direction. The main result of this section is that when $\|\boldsymbol{\alpha}\| \neq 0$, this neutral direction perturbs to either a stable or unstable direction, and precisely which is determined by the frequency map. The proof follows the strategy in Bridges (1997), but the idea of embedding the multi-symplectic PDE in a gradient flow is new.

Theorem 7.1. *Suppose there is equality in (7.4). Then for* $|\lambda| + \|\boldsymbol{\alpha}\|$ *sufficiently small, the only branch of spectra of (7.3) near* $\lambda = \boldsymbol{\alpha} = 0$ *is of the form*

$$\lambda = -\frac{1}{\|\hat{Z}\|_{1,2}^2} \left\langle \boldsymbol{\alpha}, \left(\frac{\delta \boldsymbol{\omega}}{\delta I}\right)^{-1} \boldsymbol{\alpha} \right\rangle + o(\|\boldsymbol{\alpha}\|^2). \tag{7.5}$$

$\|\cdot\|_{1,2}$ *is the* $H^1(\mathbb{S}^1, \mathbb{V}^{\mathbb{C}})$ *norm. The angle brackets in (7.5) represent a standard real inner product on* $\mathbb{R}^n$.

Remark 7.2. In the case $n=1$, this result reduces to

$$\lambda = -\frac{1}{\|\hat{Z}\|_{1,2}^2} \omega'(I)^{-1} \alpha^2 + o(|\alpha|^2).$$

In this case, the sign of $\omega'(I)$ determines whether the perturbed neutral direction changes to a stable or unstable direction.

Proof. The proof is a straightforward application of the Lyapunov–Schmidt reduction (cf. Diemling 1985, §6.2). Let $\boldsymbol{P}$ be a projection onto the kernel of $\boldsymbol{L}$, then the spectral problem (7.3) is equivalent to

$$\left.\begin{aligned} (\boldsymbol{I}-\boldsymbol{P})\boldsymbol{L}U &= (\boldsymbol{I}-\boldsymbol{P})\Big(\lambda U + \sum_{j=1}^{n} \mathrm{i}\alpha_j \boldsymbol{J}_j U\Big), \\ 0 &= \lambda \boldsymbol{P} U + \sum_{j=1}^{n} \mathrm{i}\alpha_j \boldsymbol{P}\boldsymbol{J}_j U, \end{aligned}\right\} \tag{7.6}$$

since $\boldsymbol{P}\boldsymbol{L}=0$. The first equation can be solved to leading order by noting that

$$\boldsymbol{L}\left(\frac{\partial \hat{Z}}{\partial \omega_j}\right) = \boldsymbol{J}_j \hat{Z}_\theta = \nabla A_j(\hat{Z}), \quad j = 1, \ldots, n.$$

Hence, it follows that

$$U(\theta) = \mathbb{C}\left(\hat{Z}_\theta + \sum_{j=1}^{n} \mathrm{i}\alpha_j \hat{Z}_{\omega_j}\right) + \mathcal{O}(|\alpha|^2),$$

is a solution of the first equation of (7.6) to leading order, with $\mathbb{C}$ a complex constant. Substituting this leading order expression into the second equation of (7.6) results in

$$\mathbb{C}\left(\|\hat{Z}\|_{1,2}^2 \lambda + \sum_{j=1}^{n}\sum_{k=1}^{n} \alpha_j \alpha_k \oint \langle\langle \boldsymbol{J}_j \hat{Z}_\theta, \hat{Z}_{\omega_k} \rangle\rangle \mathrm{d}\theta\right) + o(|\alpha|^2) = 0.$$

The result (7.5) then follows by noting that

$$\frac{\partial}{\partial \omega_k} \mathcal{A}_j(\hat{Z}) = \oint \langle\langle \boldsymbol{J}_j \hat{Z}_\theta, \hat{Z}_{\omega_k} \rangle\rangle \mathrm{d}\theta,$$

and that the matrix $\delta\mathcal{A}/\delta\boldsymbol{\omega} = (\delta\boldsymbol{\omega}/\delta I)^{-1}$. ■

When $\boldsymbol{\alpha}\neq 0$ the perturbation of the neutral direction is determined by the signs of the n eigenvalues of the symmetric matrix $\delta\boldsymbol{\omega}/\delta I$. The result is curious because $\boldsymbol{\alpha}\neq 0$ enlarges the function space in which the gradient flow is being studied. To see this latter point, consider the solution $\hat{U}(\theta, x, t)$ of the linearized system (7.2) and restrict x to one dimension. It can be written in the form

$$\hat{U}(\theta, x, t) = \mathrm{Re}(\mathrm{e}^{\lambda t + \mathrm{i}\alpha x_1} U(\omega_1 x_1 + \theta_0)),$$

(simplifying the representation of the inverse Fourier transform for brevity). This solution is not periodic of period $2\pi/\omega_1$ in general unless $\alpha = 0$. In other words, the effect of the frequency map on the gradient flow only shows up when the space of functions in the analysis of the gradient flow is enlarged from $L^2(\mathbb{S}^1, \mathbb{V}^{\mathbb{C}})$ to $L^2(\mathbb{R}, \mathbb{V}^{\mathbb{C}})$.

(*a*) *Towards a generalization of Morse–Floer theory*

The above results are linear but they show that some results can be obtained by embedding multi-symplectic elliptic PDEs in a gradient flow. There is evidence in the literature that encourages the idea of a full generalization of Floer theory to multi-symplectic PDEs. Results of Angenent & Van Der Vorst (1999, 2000) extend Floer theory to elliptic PDEs of the form (1.10). An indication of how this theory can be multi-symplectified is given here.

First, as shown in §1, systems like (1.10) are easily multi-symplectified, and the elliptic system (1.7) can be obtained formally as the first variation of the Lagrangian

$$\int_M \mathcal{L}_S, \quad \mathcal{L}_S(Z) = \Theta(Z) - S(Z)\mathrm{d}\mathcal{V}. \tag{7.7}$$

Hence, in an appropriate space of functions, solutions of the elliptic PDE (1.7) can be characterized as critical points of this functional. The L_2-gradient flow associated with $\mathcal{L}_S$ is of the form (7.1).

A generalization of Morse–Floer theory would proceed as follows. Choose a space of functions (say a Sobolev space of periodic or multi-periodic functions) on which $\mathcal{L}_S$ has critical points. Let $\hat{Z}_\pm$ be any two distinct such critical points and place $\hat{Z}_\pm$ at $t = \pm\infty$.

Let $\hat{Z}_+$ and $\hat{Z}_-$ be two distinct solutions in the chosen class. Then the idea is to study the connecting orbits between these two states in the gradient flow with

$$\lim_{t\to\pm\infty} Z(x, t) = \hat{Z}_\pm(x).$$

A critical step would then be to establish whether the linearization of the gradient flow about a connecting orbit is Fredholm, in a suitable class of functions, and determine its index. The functional analysis required for establishing this property should not be too different from that used in the analysis of the nonlinear Dirac equation (e.g. Gilbert & Murray 1991; Esteban & Séré 2002).

If the linearization of the gradient flow about a connecting orbit is Fredholm, it raises the following question. Does there exist an index associated with the states at infinity $\hat{Z}^\pm$, such that the Fredholm index of the linearization about a connecting orbit can be expressed as the difference between the indices of the states at infinity? In other words, an index associated with critical points of

$\mathcal{L}_S(Z)$, which generalizes the Maslov index for periodic orbits of Hamiltonian systems, and the index for elliptic operators of Angenent & Van Der Vorst (2000) to abstract systems of the form (1.7).

The proposed gradient flow (7.1) is closer to the framework of Floer (1988) since the left-hand side is a generalized Cauchy–Riemann equation, whereas in Angenent & Van Der Vorst (2000) a bi-directional heat equation is studied. However, whether stronger results can be obtained by analysing the gradient flow of (7.1) rather than the gradient flow in Angenent & Van Der Vorst (1999) is an open question.

8. Hybrid multi-symplectic structures and the NLS equation

The PDEs generated by $\boldsymbol{\Theta}$ are covariant, i.e. the form of the PDE is independent of the choice of coordinates. However, in mechanics and pattern formation, one typically has covariance in space, but time is a preferred direction. Therefore, one cannot mix up space and time coordinates. Moreover, the order of derivative in time may differ from the order of derivative in space. In this setting, the multi-symplectic structure becomes stratified. In this section, an example will be used to show how such PDEs are multi-symplectified.

Consider the NLS equation with general nonlinearity introduced in (1.14) and take $x\in\mathbb{R}^2$. Setting $A_t=0$ reduces (1.14) to a covariant equation in a form where the theory of $\boldsymbol{\Theta}$ is applicable. There are a number of different ways the covariant part of (1.14) can be multi-symplectified using $\boldsymbol{\Theta}$. For example, one can consider A as vector-valued leading to $\boldsymbol{\Theta}$ on $\mathbb{R}^2\otimes\bigwedge(T^*\mathbb{R}^2)$, or one can consider A as a one form. The latter strategy is more interesting.

Let $A(x_1,x_2,t)=A_1(x_1,x_2,t)+\mathrm{i}A_2(x_1,x_2,t)$, and consider the components of A as components of a differential form on $M=\mathbb{R}^2$, i.e. a section of $\boldsymbol{\Omega}^1(M)$ parameterized by time,

$$\boldsymbol{u}(x_1,x_2,t) := A_1(x_1,x_2,t)\mathrm{d}x_1 + A_2(x_1,x_2,t)\mathrm{d}x_2.$$

In terms of this one form, the NLS equation can be reformulated as

$$\begin{aligned} \delta\boldsymbol{u} &= \phi, \\ \star\boldsymbol{u}_t + \mathrm{d}\phi + \delta v &= V'(|\boldsymbol{u}|^2)\boldsymbol{u}, \\ \mathrm{d}\boldsymbol{u} &= v, \end{aligned}$$

where $\phi\in\boldsymbol{\Omega}^0(M)$, $\boldsymbol{v}\in\boldsymbol{\Omega}^2$ and $\star$ is the Hodge star operator, or

$$\boldsymbol{m}Z_t + \boldsymbol{J}_{\boldsymbol{\partial}}Z = \nabla S(Z),$$

where $\boldsymbol{J}_{\boldsymbol{\partial}}$ is the usual multi-symplectic Dirac operator on $\mathbb{R}^2$, $Z=(\phi,\boldsymbol{u},\boldsymbol{v})$,

$$S(Z) = \tfrac{1}{2}\star(\phi\wedge\star\phi + v\wedge\star v + V(\|\boldsymbol{u}\|^2)\mathrm{d}\mathcal{V}),$$

and

$$\boldsymbol{m} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \star & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}.$$

The multi-symplectic structure is composed of two parts: the standard $\boldsymbol{J}_{\boldsymbol{\partial}}$ acting on sections of $\bigwedge(T^*M)$ with $M=\mathbb{R}^2$, and a symplectic structure associated with the action of $\bigstar$ on a sub-bundle of $\bigwedge(T^*M)$ with two-dimensional fibre. Analysis of this equation can proceed as in the covariant case, taking into account the special nature of the symplectic structure in time.

9. Concluding remarks

Although this paper has been restricted to elliptic PDEs, hyperbolic PDEs can also be obtained from $\boldsymbol{\Theta}$ when the Euclidean metric is replaced by a Lorentzian metric. Abstractly, the theory is similar, but there are enough differences in detail to warrant a separate treatment. For example, the kernel of $\boldsymbol{J}_{\boldsymbol{\partial}}$ will no longer be related to the harmonic forms, and the Clifford algebra structure changes.

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