CHAPTER 1

SLOW MANIFOLDS

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A key mathematical concept for the understanding of the dynamics of coherent structures in typical (as opposed to integrable) spatially extended systems is that of a slow manifold. The theory of slow manifolds is reviewed and extended here, with special emphasis on the Hamiltonian context. For a broad range of dynamical systems with a small separation of timescales parameter ε, given any integer $r \geq 1$, existence of a slow manifold and slow vector field εX on it, containing all nearby equilibria and with error field of order $(\varepsilon|X|)^r$, is proved. In the Hamiltonian case, Hamiltonian slow dynamics is constructed and the theory is extended to slow manifolds with an internal oscillation. Applications are given to a variety of problems, including the interactions of localised excitations in several types of spatially extended system. In particular, the theory helps one to understand the interaction and propagation of discrete breathers.

1. Introduction

Definition 1: A *slow manifold* for a smooth (i.e. C^k for some $k \geq 1$) vector field V on a manifold P is a smooth submanifold M together with a tangential vector field U on it (called the *slow vector field*), such that

(1) U is close to V on M,
(2) in local coordinates $(x, y) \in M_j \times E$, where $\bigcup_j M_j$ is an open cover of M and E is a Banach space (complete normed linear space) representing displacements from M, and writing $V = (u, v)$ in these coordinates, then $||\,(\partial v/\partial y)^{-1}\,||$ is small compared to significant timescales for the system $\dot{x} = U(x)$ on M (say the time for $V - U$ to change by an order-one factor along the orbits of U).

If $U = V$ on M then M is an *invariant* slow manifold (some authors add this to the definition of slow manifold but it will be seen to be too restrictive).

Sometimes I am sloppy in the use of the term "slow manifold" and mean just M rather than the pair (M, U). The ambient space P may be infinite-dimensional, in which case M may be of infinite dimension or codimension.

For example, systems of the form

$$\begin{aligned} \dot{x} &= \varepsilon X(x, y) \\ \dot{y} &= Y(x, y) \end{aligned} \tag{1}$$

for ε small have a slow manifold $M = \{(x, y) : Y(x, y) = 0, ||(\partial Y/\partial y)^{-1}|| \ll 1/\varepsilon\}$, which is locally a graph $y = \eta(x)$ (by the implicit function theorem), carrying slow dynamics $\dot{x} = \varepsilon X(x, \eta(x))$.

The main advantage of finding a slow manifold is *dimension reduction*: all the fast variables are eliminated by "slaving" to the slow ones, giving a differential-algebraic system of lower order. Another advantage is improved initialisation from imperfect data: one can push the initial conditions onto the slow manifold to reduce unwanted rapid oscillations in numerical integrations. The utility of a slow manifold, however, depends on its accuracy, so it can be important to find accurate ones.

Much has been written about slow manifolds. They are fundamental to relaxation oscillators, slaving effects, the realisation of holonomic constraints, and interactions of coherent structures. The main mathematical issues are:

(1) given a candidate slow manifold M, to determine a suitable slow vector field U on it (some projection of V),
(2) given one slow manifold M, to find a better one $\tilde{M}$, in the sense that condition (1) of the definition is satisfied more strongly,
(3) to decide whether or not an invariant slow manifold exists, i.e. one for which V is everywhere on M tangent to M, and so U can be taken to be simply the restriction of V to M.
(4) to decide for how long true orbits remain close to those of the approximate dynamics on the slow manifold.

I will work with systems like Eq. (1) where the fast motion happens on timescales of order 1 and the slow timescale is long $(1/\varepsilon)$. Many systems of different forms, however, can be treated similarly, or put into this form by change of variables, e.g. the van der Pol oscillator in the relaxation regime is usually written as

$$\begin{aligned} y_1' &= -x_1 \\ x_1' &= y_1 - \lambda(x_1^3/3 - x_1), \qquad \lambda \text{ large,} \end{aligned} \tag{2}$$

but can be converted to

$$\begin{aligned} \dot{x} &= -\varepsilon y \\ \dot{y} &= x - y^3/3 + y \end{aligned} \tag{3}$$

by $\varepsilon = 1/\lambda^2$, $x = y_1/\lambda$, $y = x_1$ and the time change $\dot{z} = z'/\lambda$ for general functions z.

Although much of what follows is well known to experts, I have not found a comprehensive account in the literature which goes as far as I have; in fact, I believe some of the results here are new. Some precursors are Refs 1-5 (also Ref. 6 is a significant precursor for the sections on Hamiltonian slow manifolds with internal oscillation). In particular, it turns out that I have followed similar lines to van Kampen, but with significant extensions. For some relatively recent lists of references to slow manifolds, see Refs 7 and 8. Additional topics that I would like to cover one day are slow manifold approaches to the Born-Oppenheimer approximation in quantum dynamics of molecules (for excellent recent work on this, see Ref. 9) and to the derivation of stochastic equations of motion for slow degrees of freedom as a result of their coupling to chaotic fast ones (on which there is a large literature, e.g. Ref. 10, but for which I'm not aware of a good treatment in the Hamiltonian case).

Here is an outline of the contents. In Sections 2 and 3, I'll highlight the special features of the normally hyperbolic and Hamiltonian cases, respectively. In Section 4 I'll introduce an iterative scheme to produce r^{th} order slow manifolds from a 0^{th} order one. I'll adapt the procedure in Section 5 to produce Hamiltonian ones for Hamiltonian systems. In Sections 6 and 7 I compare my method with some precursors. Section 8 is a short aside on an extension from Hamiltonian to Poisson systems. Section 9 introduces the concept of slow manifold with internal oscillation, which is of crucial importance for a variety of applications. Theory and examples are given for $U(1)$-symmetric Hamiltonian systems in Section 10 and for general Hamiltonian systems in Section 11. Section 12 gives methods to obtain bounds on the time evolution of initial conditions on or near a slow manifold. These lecture-notes close in Section 13 with some comments on the effects of weak damping on Hamiltonian cases.

2. Normally Hyperbolic versus General Case

The theory of slow manifolds is in very good shape if there is a *normally hyperbolic* slow manifold, i.e. the spectrum of $(\partial v/\partial y)$ at all its points avoids a neighbourhood of the imaginary axis. This is the case in typical slaving problems. A textbook example is Michaelis-Menten enzyme kinetics, e.g. Ref. 11:

$$\begin{aligned}\dot{c} &= s - (s+K)c \\ \dot{s} &= \varepsilon(-s + (s+K-U)c),\end{aligned} \tag{4}$$

for which c collapses rapidly towards the slow manifold $c = s/(s+K)$, which then gives the (non-mass action) rate law $\dot{s} \approx -\varepsilon U s/(s+K)$. Another is the Fitzhugh-Nagumo model of a neuron, e.g. Ref. 11:

$$\begin{aligned}\dot{v} &= f(v) - w - w_0 \\ \dot{w} &= \varepsilon(v - \gamma w - v_0),\end{aligned} \tag{5}$$

with $f(v) = Av(v-\alpha)(1-v)$, for which v relaxes rapidly onto the attracting parts of the curve $w = f(v) - w_0$, followed by slow evolution along this curve until near a turning point.

For such problems one can do much better than just approximations. The theory of normally hyperbolic invariant manifolds[12] applies, which proves that there is a locally invariant slow manifold nearby, together with many other useful results (smoothness, persistence, forwards and backwards contracting foliations, local linearisability in the normal direction, and local maximality and uniqueness in case of full invariance; furthermore there are strong results on the approach and departure from normally hyperbolic invariant slow manifolds[13]). So exact dimension reduction is possible.

In principle, this exact dimension reduction could be used in numerics. It would be extremely useful, for example, in biochemical reaction networks, neurophysiological circuits and chemically reacting flows, where there are typically hundreds of variables but a large fraction are fast and could be eliminated. Indeed Ref. 14 discusses how to use the existence of normally hyperbolic invariant slow manifolds in numerical computations, but I think more could be done. Ref. 15 computes “intrinsic low-dimensional manifolds” (ILDM), which are “second order” slow manifolds in the terminology I will introduce, but in general not invariant[a]. There is good computational work for special cases of normally hyperbolic manifolds, e.g. local

[a]Although Deuflhardt[16] appreciates this fact, Maas's paper does not mention it, so here is an example: applied to a system of the form $\dot{x} = \varepsilon x, \dot{y} = -y + \delta(x)$, his method

unstable[17] and centre manifolds[18] of equilibria and periodic orbits, and inertial manifolds.[19,20,21] I am aware of only one paper on a computational approach to general normally hyperbolic manifolds,[22] though even this treats only discrete time systems and the case of trivialisable backwards and forwards contracting normal bundles.

In contrast, the situation is much more delicate for slow manifolds which are not normally hyperbolic. This is the case in many classical mechanical problems. For example, a pendulum on a stiff spring behaves roughly like a rigid pendulum but with possible fast oscillations in the length superposed. Similarly, the classical motion of a hydrocarbon can be regarded as slow motion of the carbon skeleton with fast oscillation of CH stretches and bends superposed. Other examples are: compressible fluid dynamics separates at low Mach number into incompressible fluid dynamics and acoustic waves (e.g. Ref. 23), water waves separate into gravity waves with surface tension ripples (e.g. Ref. 24), and many nonlinear classical field theories possess propagating coherent structures (such as kinks and monopoles) surrounded by small radiation (e.g. Refs. 25-28). Mid-latitude atmospheric dynamics provides an example of a system with three ranges of timescale: geostrophic motion on a 6-hour scale, inertia-gravity waves on a 5-minute scale, and acoustic waves on scales of a few seconds or less (e.g. Ref. 29).

For a general system with a slow manifold which is not normally hyperbolic, it is unlikely that there is an invariant slow manifold nearby, because typical smooth perturbations of a system with an invariant manifold which is not normally hyperbolic are believed to destroy it[b].

Example 2: A fragile invariant slow manifold

A simple illustration of the fragility of invariant slow manifolds is furnished by the system

$$\begin{aligned}\dot{\theta} &= \varepsilon\omega(I) \\ \dot{I} &= 0 \\ \dot{\xi} &= \eta + \delta g(\theta) \\ \dot{\eta} &= -\xi,\end{aligned} \tag{6}$$

yields ILDM $y(x) = \delta(x) - \varepsilon x\delta'(x)/(1+\varepsilon)$, on which the deviation of $\dot{y}$ from $y'(x)\dot{x}$ is $\varepsilon x^2\delta''(x)/(1+\varepsilon)$.

[b] The only precise result of this form that I know, is somewhat weaker: if for a C^1 compact invariant submanifold M for a C^1 diffeomorphism f there is a neighbourhood U of M and a neighbourhood V of f such that for all $g \in V$ the maximal invariant set for g in U is a C^1 submanifold M_g and M_g is C^1-close to M, then M is normally hyperbolic.[30]

where $\theta \in S^1 = \mathbb{R}/2\pi\mathbb{Z}$, $I \in [1,2]$, $\omega(I) = I$ (variants are possible, hence the more general notation), $\delta \in \mathbb{R}$, and $g(\theta) = \sum_{m\in\mathbb{Z}} g_m e^{\mathrm{i}m\theta}$ is a function analytic in a strip $|\Im\theta| \le \kappa$ with all Fourier coefficients g_m nonzero, e.g.

$$g(\theta) = \frac{1}{2-\cos\theta}. \tag{7}$$

The analyticity implies that $|g_m| \le Ce^{-\kappa|m|}$ with $C = \sup\{|g(\theta)| : |\Im\theta| \le \kappa\}$. The case $\delta = 0$ has an invariant slow manifold $M = \{(\theta, I, 0, 0) : \theta \in S^1, I \in [1,2]\}$. Let us seek an invariant slow manifold for $\delta \ne 0$ as a Fourier series $\xi(\theta, I) = \sum_{m\in\mathbb{Z}} \xi_m e^{\mathrm{i}m\theta}$, $\eta(\theta, I) = \sum_{m\in\mathbb{Z}} \eta_m e^{\mathrm{i}m\theta}$. The equations for each order m of Fourier coefficients separate and there is a unique solution

$$\begin{aligned} \eta_m &= \frac{\delta g_m}{m^2\varepsilon^2\omega(I)^2 - 1}, \\ \xi_m &= -\mathrm{i}m\varepsilon\omega(I)\eta_m, \end{aligned} \tag{8}$$

if the denominator is nonzero. If the denominator has a zero, however, then there is no solution. This happens where $\omega(I) = \pm 1/m\varepsilon$. Now $\omega(I)$ goes from 1 to 2, and m ranges through the whole of $\mathbb{Z}$. Thus for all $\varepsilon \le 1$, the invariant slow manifold goes to infinity at a set of $N \sim 1/\varepsilon$ values of I and there is no solution valid uniformly on $I \in [1,2]$.

Nevertheless, for this example there exists a very nearly invariant slow manifold uniform in I, e.g. for any $\alpha \in (0, 1/\omega_{\max})$, where $\omega_{\max} = 2$, define $M(\alpha)$ by

$$\eta_m = \frac{\delta g_m}{m^2\varepsilon^2\omega(I)^2 - 1} \text{ for } |m| < \frac{\alpha}{\varepsilon}, 0 \text{ otherwise}, \tag{9}$$

$$\xi_m = -\mathrm{i}m\varepsilon\omega(I)\eta_m. \tag{10}$$

The normal component of the vector field on $M(\alpha)$ is of order $\delta e^{-\kappa\alpha/\varepsilon}$, i.e. exponentially small in ε, and $M(\alpha)$ is within order δ of the unperturbed one (in any C^k).

Thus sensible goals in the general case are, given one slow manifold, (i) to try to construct a better one, i.e. one for which condition (1) of the definition holds more strongly, and (ii) to determine how small any deviations from invariance can be made. These issues will be addressed in Section 4. There are also related goals for numerical computation, which I will not address here, but some references are Refs 31-33, 8.

3. Hamiltonian versus General Case

Many potential applications of slow manifolds are Hamiltonian systems, especially most of those which are not normally hyperbolic. Recall that a *Hamiltonian system* is a vector field V on a manifold P defined by $\Omega(V,\xi) = dH(\xi)\ \forall \xi \in TP$, for some function $H : P \to \mathbb{R}$ (called the "Hamiltonian") and "symplectic form" Ω on P. A *symplectic form* is a closed ($\int_{S^2} \Omega = 0$ for all contractible 2-spheres in P), non-degenerate ($\Omega(\xi,\eta) = 0\ \forall\xi \implies \eta = 0$), antisymmetric ($\Omega(\eta,\xi) = -\Omega(\xi,\eta)$) bilinear (linear in each argument) form on the tangent space TP (Ω takes two tangent vectors at a point of P and returns a real number). The "canonical" example is $\Omega = \sum_{j=1}^{d} dq_j \wedge dp_j$ on $\mathbb{R}^d \times \mathbb{R}^d$, which gives Hamilton's equations $\dot{q}_j = \frac{\partial H}{\partial p_j}, \dot{p}_j = -\frac{\partial H}{\partial q_j}$. Ref. 34 is a good text on the differential topology formulation of Hamiltonian dynamics.

Hamiltonian systems have special properties, mostly associated with preservation of the symplectic form. So in the Hamiltonian case, one would hope to construct slow manifolds on which the slow dynamics is itself Hamiltonian, and we will see in Section 5 that this is indeed often possible.

It should be remarked that if one restricts to the Hamiltonian context, there are invariant manifolds which survive all small Hamiltonian perturbations but are not normally hyperbolic. The obvious examples are the regular energy levels, but even within an energy level there can be persistent invariant manifolds, e.g. KAM tori (*KAM tori* are invariant tori on which the motion is smoothly conjugate to a constant vector field with incommensurate direction, e.g. Refs 34, 35) and the stable and unstable manifolds of KAM tori of dimensions strictly between 1 and the number d of degrees of freedom. All the examples I know, however, are non-symplectic whereas I believe the interesting case for slow manifolds (in Hamiltonian systems) is *symplectic submanifolds*, i.e. on which the symplectic form is non-degenerate, because that condition is necessary to define a natural Hamiltonian dynamics on them. It would be a good project to try to prove a generic non-persistence result for symplectic submanifolds of Hamiltonian systems (but without requiring the local maximality of Ref. 30). A result in this direction was obtained by Fermi (see Ref. 36 for an appraisal). In the context of infinite-dimensional systems exhibiting coherent structures and radiation, Ref. 29 suggests that such a result should follow from the fact that typical motions of coherent structures generate radiation; an initial context in which to address this might be kinks moving in a lattice, e.g. Ref. 37. Perhaps the variational principle of Ref. 38 could be useful to make a general proof.

As a start, it would be interesting to study the following Hamiltonian version of Example 2, for which I give the beginnings of an analysis.

Example 3: A fragile Hamiltonian invariant slow manifold

Let $H(I,\theta,\xi,\eta) = \frac{\varepsilon}{2}I^2 + \frac{1}{2}(\xi^2+\eta^2) + \delta g(\theta)\eta$ and $\Omega = d\theta \wedge dI + d\xi \wedge d\eta$, where $\theta \in S^1$, $I \in [1,2]$, $\xi, \eta \in \mathbb{R}$, $\delta \in \mathbb{R}$ and g is an analytic function in a strip $|\Im\theta| \leq \kappa$. For $\delta = 0$ there is an invariant slow manifold $\xi = \eta = 0$. It consists of periodic orbits given by $I =$ constant, of period $2\pi/\varepsilon I$. Their Floquet multipliers are $\exp \pm 2\pi \mathrm{i}/\varepsilon I$. Given $\beta > 0$ there is a $\delta_0(\varepsilon,\beta) > 0$ such that the periodic orbits with Floquet multipliers at least β from $+1$ persist for $|\delta| \leq \delta_0$ (moving by at most order $|\delta|/\beta\varepsilon$), so the parts of the invariant slow manifold where $|I - \frac{1}{m\varepsilon}| \leq \frac{\beta}{m^2\varepsilon}$ survive such perturbation. These form $N \sim 1/\varepsilon$ invariant annuli (for $\beta < 1/2$). Generic Hamiltonian perturbation, however, destroys periodic orbits with a Floquet multiplier $+1$, so we can expect the family of periodic orbits to be punctured around $I = 1/m\varepsilon$ for each $m \in \mathbb{Z}$. When $\delta = 0$, the set of periodic orbits near $I = 1/m\varepsilon, \xi = \eta = 0$, of period near $2\pi/\varepsilon I$, is (modulo rotation in θ) the union of the line $\xi = \eta = 0$ and the plane $I = 1/m\varepsilon$. The perturbation δ can be expected to turn this into a broken pitchfork, as shown in Figure 1(a-b). Taking all integers m between $1/2\varepsilon$ and $1/\varepsilon$ yields a "ladder" of broken pitchforks as in Figure 1(c). The same phenomenon occurs in classical models of stretches of water molecules (as was observed by Mark Child and explained by me in similar terms in 1993, though never published; see Ref. 39, however, for related numerics).

One might ask whether there could still be an invariant slow manifold C^1-close to the unperturbed one, without the gaps, but the answer is no, because it would be symplectic, two-dimensional and without equilibria, so the motion on it would be Hamiltonian of one degree of freedom and consist entirely of periodic orbits of nearby period. One can connect the invariant annuli, however, into an almost invariant slow manifold: any surface C^1-close to $\xi = \eta = 0$ and connecting the invariant annuli will do, such as the dotted curve in Figure 1(c).

To examine whether the specific perturbation by δ above really punctures the family of periodic orbits, and how close to invariant one can make a slow manifold, one would have to do a more detailed calculation. Here is a sketch.

Near $I = 1/m\varepsilon, \xi = \eta = 0$, use coordinates (x,y), defined by $x + iy = (\xi + i\eta)e^{im\theta}$, and $K = I - 1/m\varepsilon + \frac{m}{2}r^2$, where $r^2 = x^2 + y^2$. Then $H = \frac{1}{2m^2\varepsilon} + 2K/m + \frac{\varepsilon}{2}(K - \frac{m}{2}r^2)^2 + \delta g(\theta)\Im(e^{-im\theta}(x+iy))$ and $\Omega = d\theta \wedge dK + dx \wedge dy$. This is in a suitable form to apply the method of averaging (e.g. Ref. 40), i.e. a near-identity coordinate change to reduce the θ-dependence of H while keeping the same expression for Ω. Using the

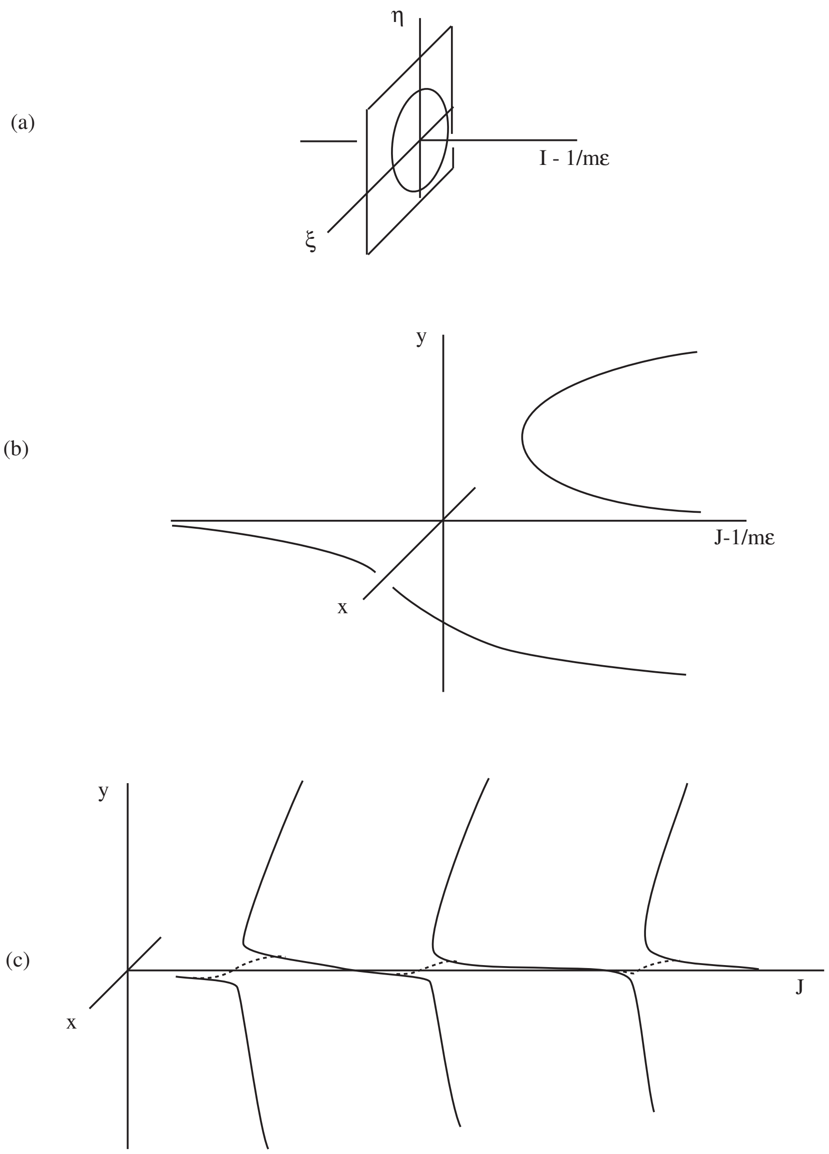

Fig. 1. Expected effect of δ on the set of periodic orbits near $I = 1/m\varepsilon, \xi = \eta = 0$ with period near $2\pi/\varepsilon I$: (a) $\delta = 0$, (b) $\delta \neq 0$, where (x, y) are coordinates rotating in the (ξ, η)-plane at rate m with respect to θ, and $J = I + \frac{x^2+y^2}{2\varepsilon I}$, (c) part of the resulting ladder of broken pitchforks and an example of a way to make an almost invariant slow manifold (dotted curve).

same symbols for the new coordinates, but rotating in the (x, y)-plane if necessary, the Hamiltonian takes the form $H = \bar{H} + \tilde{H}$, with $\bar{H}$ independent of θ, $\bar{H} \approx \frac{1}{2m^2\varepsilon} + 2K/m + \frac{\varepsilon}{2}(K - \frac{m}{2}r^2)^2 + f(\delta)y$ for some f which goes to 0 with δ and is of size at most order $e^{-\kappa m}$, and the gradient of $\tilde{H}$ is of smaller order. Note that the above form for $\bar{H}$ is already obtained in one iteration of the averaging method (with $f(\delta) = \delta|g_m|$), but further iterations are required to reduce $\tilde{H}$ to smaller order, and in general the iterations introduce additional terms of the same order into f.

Let us first analyse the dynamics of $\bar{H}$. Since $\bar{H}$ is independent of θ, its dynamics conserve K, so we can study the dynamics in (x, y) as a function of K. Its equilibria are given by $x = 0, \frac{\varepsilon}{2}m^2y^3 - \varepsilon mKy + f = 0$, whose solutions look like Figure 1(b) for $f \neq 0$ ($K \sim J - \frac{1}{m\varepsilon}$). The rest of the dynamics consists of periodic orbits around the elliptic critical points and separatrices of the saddle, as shown in Figure 2.

No curve connecting the two branches with r small is invariant; the normal component of the vector field reaches order f somewhere in between. Nevertheless, connecting curves can be chosen so that the normal component does not exceed this size (indeed, any connecting curve with $|r| \leq (2f/m^2\varepsilon)^{1/3}$ and small slope will do), thus giving an exponentially accurate slow manifold. The effects of $\tilde{H}$ do not change this conclusion, though they fuzz out the dynamics of $\bar{H}$, because K is not exactly conserved. H is still conserved, however, and thus Figure 2 changes to a one-parameter family of surface of section plots (at say $\theta = 0$, parametrised by H), with the principal changes being that the separatrices of the saddle become stochastic layers, and invariant circles with near-rational winding ratio become zones of instability.

Ref. 41 treats numerically a similar example, proposed in Refs 42 and 43, and claims existence of an invariant "fractal slow manifold" by appealing to KAM theory, but in my opinion the existence problem has nothing to do with KAM theory, just persistence of periodic orbits, and the authors are incorrect to say that one has to avoid all rational resonances not just integer ones, so in fact their system has an invariant slow manifold consisting of a collection of annuli, as above; they are correct, however, that KAM theory can be used in their example to bound the distance orbits can go from the slow manifold and to establish nonlinear stability of large parts of it. For some analysis of this model, see Ref. 44. Another related example was studied in Ref. 45, where results closely analogous to mine were obtained independently, and also illustrated by some nice numerics. Note that most

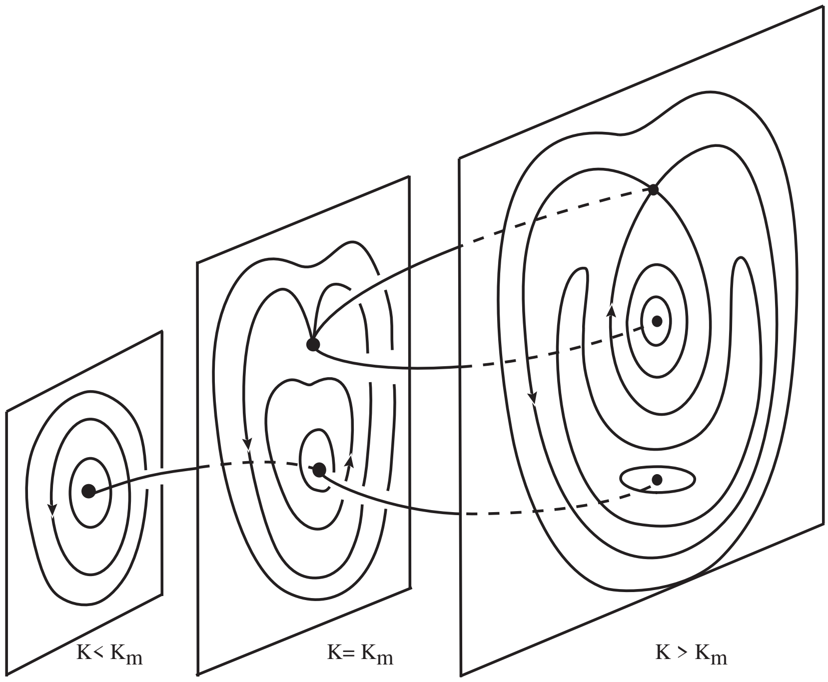

Fig. 2. The dynamics of $\bar{H}$ in the (x,y)-plane for Example 3 for three values of K. The bifurcation value $K_m \sim \frac{3m}{2}(\frac{2f}{m^2\varepsilon})^{2/3}$, and the equilibria occur at $y \sim \frac{f}{m\varepsilon K}$ for $K \ll -K_m$, $y \sim (\frac{2f}{m^2\varepsilon})^{1/3}$ and $-2(\frac{2f}{m^2\varepsilon})^{1/3}$ for $K = K_m$, and $y \sim \frac{f}{m\varepsilon K}$ and $\pm\sqrt{\frac{2K}{m}}$ for $K \gg K_m$.

orbits of Hamiltonian slow dynamics on any 2D symplectic submanifold are periodic, because it is a 1 degree of freedom Hamiltonian system (so every regular compact connected component of a level set is a periodic orbit), which confirms Lorenz's intuition.

Another special context worth mentioning for slow manifolds is families of Hamiltonian systems perturbed weakly, but not necessarily Hamiltonianly, by slow evolution of the parameters of the family, studied in Ref. 46.

Returning to the Hamiltonian context, with normally elliptic behaviour it is natural to try to go beyond just finding good slow manifolds, by seeking to describe all the dynamics in a neighbourhood of a slow manifold. If there is just one fast degree of freedom, this is provided by the standard theory of adiabatic invariants (e.g. Ref. 35), and indeed the dynamics can be reduced by an excellent approximation to a 1-parameter family of slow Hamiltonian systems, parametrised by the adiabatic invariant for the fast degree of freedom. Extension to more than one fast degree of freedom introduces problems with resonances between them, e.g. Refs. 2, 40, 35. Nevertheless, following initial ideas of Ref. 6, I have derived a good theory for slow manifolds with one internal oscillation, irrespective of the number of other fast degrees of freedom, subject just to non-resonance of the internal oscillation with the set of linearised frequencies for the other fast modes. This is described in Sections 9–11.

4. Improving a slow manifold

This section treats the question of how much a general slow manifold can be improved in a general dynamical system. Condition (1) of my definition of slow manifold requires only that the error field $V - U$ be small, but I show that by changing the slow manifold a little one can make it include all nearby equilibria and make the error field small compared to U. Iterating the procedure makes the error field of order U^r for any $r \in \mathbb{N}$ (though perhaps with a prefactor that grows with r).

Theorem 4: Every sufficiently good slow manifold can be improved to one which contains all nearby equilibria and has small angle to the vector field.

Definition 5: I call a slow manifold with these properties *first order*.

Proof: Treat the local situation first. So we can take local coordinates $(x, y) \in M_j \times E$ on P, for some open subset $M_j \subset M$ and Banach space E, and start from

$$\begin{aligned} \dot{x} &= \varepsilon X(x, y) \\ \dot{y} &= A(x)y + \delta(x) + R(x, y), \end{aligned} \tag{11}$$

with $||A(x)^{-1}|| \leq K$ of order 1, $||\delta||_{C^1} \leq \delta_1$ small, and $R(x, y) = O(y^2)$. The equation

$$A(x)\eta + \delta(x) + R(x, \eta) = 0 \tag{12}$$

has a locally unique solution $\eta(x) \approx -A(x)^{-1}\delta(x)$. In particular, all nearby equilibria are contained in the graph $y = \eta(x)$. Then put $y = Y + \eta(x)$ to obtain

$$\dot{Y} + \varepsilon D\eta(x)X(x, Y + \eta) = A(x)Y + R(x, Y + \eta) - R(x, \eta). \tag{13}$$

Define $\tilde{X}(x,Y) = X(x, Y+\eta(x))$, $\tilde{A}(x) = A(x) + \frac{\partial R}{\partial y}(x,\eta) - \varepsilon D\eta \frac{\partial X}{\partial y}(x,\eta)$ and $\tilde{\delta}(x) = -\varepsilon D\eta(x) X(x,\eta(x))$ to obtain

$$\begin{aligned} \dot{x} &= \varepsilon \tilde{X}(x,Y) \\ \dot{Y} &= \tilde{A}(x)Y + \tilde{\delta}(x) + \tilde{R}(x,Y), \end{aligned} \tag{14}$$

where $\tilde{R} = O(Y^2)$. The term $\tilde{\delta}$ has size of order $\varepsilon|X(x,\eta(x))|\delta_1$, so the angle between the new slow manifold and the vector field is of order $\varepsilon\delta_1$.

To make the result global, we need to face the fact that there might be no diffeomorphism from $M \times E$ to a neighbourhood of M, e.g. P a Möbius band and M a circle which goes once round P, or $P = \mathbb{C}P^N$ (*complex projective space*, the set of ratios $z_0 : z_1 : \ldots : z_N$ of non-zero $(N+1)$-tuples of complex numbers) and M the subset where $z_2 = \ldots = z_N = 0$ (which will occur in Example 14). Here is one way to proceed, though one might want to improve on it for explicit calculations.

Choose a transverse foliation to M in a neighbourhood, i.e. a decomposition $\bigcup_{x\in M} F_x$ of a neighbourhood of M into smoothly varying smooth submanifolds F_x such that the tangent space T_xP at each point $x \in M$ decomposes as $TF_x \oplus T_xM$. This can be done by choosing any normal bundle and a "spray" (e.g. the geodesic spray of a Riemannian metric) and extending the normal bundle to a neighbourhood using the spray (the tubular neighbourhood theorem, e.g. Ref. 47). Choose local trivialisations of the foliation (i.e. coordinates $(x,y) \in M_j \times E$ for an open cover $\bigcup_j M_j$ of M and Banach space E, so that F_x is the subset with first coordinate x and M is $y = 0$), so we can say what $\dot{y}$ means in each of these, defining vector fields V_x^j on the leaf F_x for each j such that $x \in M_j$. Choose a partition of unity for M, i.e. a set of functions $\phi_j : M \to \mathbb{R}$ such that $\phi_j = 0$ outside M_j and $\sum_j \phi_j(x) = 1\ \forall x \in M$, e.g. Ref. 47. Then study the vector field $V_x = \sum_j \phi_j(x) V_x^j$ on each leaf F_x. It is still of the form $A(x)y + \delta(x) + R(x,y)$ in any of the local trivialisations, so has a locally unique zero $y = \eta(x)$. Since it is unique it gives the same point (even though with different coordinates) in all the coordinate systems j for which $x \in M_j$. Thereafter one continues as in the local case. □

Definition 6: A slow manifold is r^{th} *order* if it contains all nearby equilibria and the normal component of the vector field is of order the r^{th} power of the tangential component on it.

Theorem 7: If the vector field is C^r for some $r > 1$, the above procedure can be iterated, reducing the size of the normal component of the vector field to order $(\varepsilon|X(x,\eta(x))|)^r\delta_r$, where δ_r is a C^r norm of δ, giving an r^{th} order slow manifold.

For an r^{th} order slow manifold with $r>1$, the approximation is especially good near equilibria. In particular, the linearisation about an equilibrium is an exact subsystem of the full linearised dynamics as soon as $r\geq 2$.

The possibility of reducing the error to $O(\varepsilon^r)$ is standard folklore (among those who know it!), but I feel the improvements to $O((\varepsilon|X|)^r)$ and including all nearby equilibria are significant (unless $|X|$ is bounded away from zero, of course, when the two are equivalent). Firstly they give extra accuracy near equilibria, and secondly in problems like the interaction of widely separated localised coherent structures (where there may be no explicit ε or δ parameters but they could be introduced by scaling) the first improvement gives extra accuracy for large separation. One could argue that the difference between the two results is trivial because by restricting attention to a neighbourhood N of an equilibrium the effective value of ε is reduced to $\varepsilon\sup_{x\in N}|X(x)|$, but one would first have to show that one could make the slow manifold contain all nearby equilibria, and the point that one can obtain position dependent accuracy which improves near equilibria does not seem to have been made before, as far as I am aware.

The above process of improving a slow manifold involves bounding a derivative each time, however, so an r-dependent prefactor arises in the error bound, which means that in general the error can not be reduced arbitrarily for given ε by increasing r. Nevertheless, if the system is analytic, one should be able to obtain reduction of the error to something of the form $\exp -C/(\varepsilon|X(x,\eta(x))|)$, for example by applying the Neishtadt-Nekhoroshev method[48,49] of estimation of the prefactor to determine an optimal number of iterations as a function of $\varepsilon|X|$. Reduction of the error to $O(\exp -C/\varepsilon)$ has been achieved for analytic systems in the case of graphs,[50] but without the crucial factor $|X|$.

5. Symplectic slow manifolds

For Hamiltonian systems, there is extra structure, namely the symplectic form Ω. Thus it is natural to ask for slow manifolds on which the slow dynamics is also Hamiltonian. This more or less requires the slow manifold to be symplectic, i.e. the symplectic form restricted to its tangent space is non-degenerate, else one would have to invent a relevant symplectic form on it from some other considerations, or perhaps make do with a Poisson structure (I'll discuss this option in Section 8). So in this section we'll study symplectic slow manifolds.

Suppose we have a state space P with a symplectic form Ω and a Hamiltonian H, and a symplectic submanifold M of P. The Hamiltonian vector field V is defined by $\Omega(V, \xi) = dH(\xi)$ for all tangent vectors ξ. The submanifold M comes with a natural Hamiltonian vector field U tangent to it, given by $\Omega_M(U, \xi) = dH_M(\xi)$ for all $\xi \in TM$, where Ω_M and H_M are the restrictions of Ω and H to M. In nineteenth century language, U gives the equations of motion when "workless constraint forces" are applied to keep the state on M. So we will choose U for the dynamics on M. We assume that the pair (M, U) satisfies the condition for a slow manifold. We want to improve M as in the previous section to a slow manifold $\tilde{M}$ which contains all nearby equilibria and has small angle to the vector field, but keeping Hamiltonian dynamics on it.

Choose a *symplectically orthogonal foliation* F to M, i.e. a decomposition of a neighbourhood of M into smoothly varying smooth submanifolds F_z labelled by points $z \in M$, such that $z \in F_z$ and the tangent space to P at each point $z \in M$ decomposes as $TP_z = TF_z \oplus T_zM$ and

$$\Omega(\xi, \eta) = 0 \ \forall \xi \in TF_z, \eta \in T_zM. \tag{15}$$

One concrete way to make such a foliation is to construct the symplectically orthogonal bundle to M, uniquely defined at each of its points by (15), and extend it to a neighbourhood by affine subspaces in local coordinates (one would need to ensure that the overlap maps in the intersection of different charts are affine too); this gives a foliation of any neighbourhood smaller than the smallest radius of curvature of M. A more sophisticated but perhaps less implementable way is to choose a spray on P, as in the general case, and extend the symplectically orthogonal bundle to a foliation of a neighbourhood of M by the spray. The use of symplectically orthogonal projection to describe slow dynamics in Hamiltonian systems was proposed independently about the same time as me by the author of Ref. 28 (in a PDE context; in addition he addressed the many technical issues that arise there such as choice of suitable function spaces and existence of solutions).

The normal motion being fast corresponds to $||(D^2H|_{F_z})^{-1}|| \leq K$ for some K of order 1, and V close to TM corresponds to $|DH_z| \leq \delta$ for some δ small. Thus by the implicit function theorem there exists a locally unique critical point $\tilde{z}(z)$ of $H|_{F_z}$, and it depends smoothly on $z \in M$. Hence we obtain a C^1-close submanifold $\tilde{M}$ of constrained critical points of H; in particular it contains all nearby true critical points of H. Note that in contrast to the general case, we did not need trivialisations and a partition of unity, because we are looking only for a critical point of a function on each leaf, not a zero of a projection of a vector field. Since $\tilde{M}$ is C^1-close to M, $|\Omega(\xi,\eta)| \le K\delta_1|\xi||\eta|$ for $\xi \in T\tilde{M}, \eta \in TF_z$, where δ_1 is the C^1 norm of $DH|_M$. Furthermore, the restriction $\Omega_{\tilde{M}}$ of Ω to $\tilde{M}$ remains non-degenerate. Let $H_{\tilde{M}}$ be H restricted to $\tilde{M}$ and define U by $\Omega_{\tilde{M}}(U,\xi) = dH_{\tilde{M}}(\xi)$ for all $\xi \in T\tilde{M}$.

We now prove that $V - U$ is small compared to U. Firstly, $\Omega(V,\xi) = dH(\xi)$ for all ξ. In particular, for $\xi \in T\tilde{M}, \Omega(V,\xi) = dH_{\tilde{M}}(\xi) = \Omega(U,\xi)$; and for $\xi \in TF_z, \Omega(V,\xi) = dH(\xi) = 0$ and $\Omega(U,\xi) = O(\delta_1|U||\xi|)$. So $\Omega(V-U,\xi) = 0$ for all $\xi \in T\tilde{M}$ and is $O(|U|\delta_1|\xi|)$ for all $\xi \in TF_z$. It follows that $V - U = O(|U|\delta_1)$, as claimed.

For a C^r system, this procedure can be iterated to reduce the error to $O(\delta_r|U|^r)$, where δ_r is the C^r norm of $DH|_M$. In the analytic case I expect it is possible to reduce the error to $O(\exp -C/|U|)$, for example by truncation of the iteration at optimum order. This was achieved for the case of just one fast degree of freedom in Ref. 7, but without ensuring that the slow manifold contains all nearby equilibria and with error estimate only $O(\exp -C/\varepsilon)$ with $\varepsilon = \sup_{x\in M}|U(x)|$, rather than pointwise.

Note that it is not necessary to choose the foliation to be exactly symplectically orthogonal; deviations of the same order as the change from M to $\tilde{M}$ can be allowed and will still give the same order of improvement.

Now I give some examples, worked out to various stages of completeness.

Example 8: The Spring Pendulum

This consists of a light spring with one end fixed but free to rotate about it in a vertical plane, and a mass m on the other end, moving in the plane under the influence of the spring and gravity g. It has Hamiltonian

$$H(x,y,p_x,p_y) = \frac{1}{2m}(p_x^2 + p_y^2) + mgy + \frac{k}{2}(r-a)^2, \qquad (16)$$

where (x,y) denote horizontal and vertical components of position of the mass relative to the fixed end of the spring, $r = \sqrt{x^2+y^2}$, and (p_x,p_y) the components of its momentum. The symplectic form Ω is the canonical one

$dx \wedge dp_x + dy \wedge dp_y$. The equations of motion are:

$$\begin{aligned}
\dot{x} &= \frac{p_x}{m} \\
\dot{y} &= \frac{p_y}{m} \\
\dot{p}_x &= -k(r-a)\frac{x}{r} \\
\dot{p}_y &= -mg - k(r-a)\frac{y}{r}.
\end{aligned} \tag{17}$$

The parameter regime of interest is g small. Then there is an obvious symplectic slow manifold M_0 corresponding to the spring length being fixed to a. Parametrised by the angle θ of the pendulum to the downward vertical and the angular momentum $p_\theta = xp_y - yp_x$, M_0 can be expressed as:

$$\begin{aligned}
x &= a \sin\theta \\
y &= -a\cos\theta \\
p_x &= \frac{1}{a}\cos\theta \; p_\theta \\
p_y &= \frac{1}{a}\sin\theta \; p_\theta.
\end{aligned} \tag{18}$$

One computes that $\Omega_{M_0} = d\theta \wedge dp_\theta$ and $H_{M_0} = \frac{1}{2ma^2}p_\theta^2 - mga\cos\theta$, so the zeroth order slow dynamics is simply that of a rigid pendulum. It is slow (a typical inverse time is $\sqrt{g/a}$) compared to the frequency (of order $\sqrt{k/m}$) for the linearised normal motion, provided $p_\theta = O(\sqrt{g})$, so it is sensible to write $p = \sqrt{g}P$ and work with P instead of p. One can check that in (x, y, P_x, P_y) coordinates the error vector field is small (order $\sqrt{g}$), but this is of the same size as the vector field of H_{M_0}, so the approximation is not reliable enough. Furthermore, M_0 does not contain the equilibria of the spring pendulum, which are at $x = p_x = p_y = 0$, $y = \pm a - \frac{mg}{k}$. So we will compute a first order symplectic slow manifold.

For symplectically orthogonal foliation, choose the leaves F_{θ,p_θ} defined by

$$\begin{aligned}
x\cos\theta &= y\sin\theta \\
xp_y - yp_x &= p_\theta.
\end{aligned} \tag{19}$$

They can be parametrised by (r, p_r), the radius and radial momentum ($p_r = (xp_x + yp_y)/r$). Then $H = \frac{1}{2m}(\frac{p_\theta^2}{r^2} + p_r^2) - mgr\cos\theta + \frac{k}{2}(r-a)^2$. So making H critical on F_{θ,p_θ} yields the first order symplectic slow manifold M_1 defined by $p_r = 0$ and $r = \rho(\theta, p_\theta)$, the root of $\frac{p_\theta^2}{mr^3} + mg\cos\theta = k(r-a)$ near a.

Then

$$H_{M_1} = \frac{p_\theta^2}{2m\rho(\theta, p_\theta)^2} - mg\rho(\theta, p_\theta)\cos\theta + \frac{k}{2}(\rho(\theta, p_\theta) - a)^2 \tag{20}$$

and $\Omega_{M_1} = d\theta \wedge dp_\theta$ still (because $p_r = 0$). The resulting slow vector field U is $\dot\theta = \frac{p_\theta}{m\rho^2}$, $\dot p_\theta = mg\rho\sin\theta$. Computing the error vector field $V - U$ on M_1, one finds its components to be $\dot\theta = 0$, $\dot p_\theta = 0$, $\dot p_r = 0$, $\dot r = -\frac{gp_\theta \sin\theta}{k\rho^2 + 3p_\theta^2/m\rho^2}$, and so bounded by the quadratic expression $\dot\theta \dot p_\theta / k\rho$ in the components of the slow vector field, confirming that M_1 is a first order slow manifold, and showing that it is actually second order. This fluke arises because M_1 happens to still be symplectically orthogonal to the foliation (as $p_r = 0$ on M_1).

Since M_1 is a second order slow manifold, one can in particular obtain the exact slow part of the linearised dynamics about the equilibria by taking the quadratic part of $H|_{M_1}$ there (note that the third term of (20) contributes to this).

Example 9: Interaction of kinks

For a nonlinear wave equation $u_{tt} = u_{xx} - V'(u)$ with V possessing (at least) two minima at the same height, a *kink* is a solution asymptotic to one minimum as $x \to -\infty$ and to a minimum with a larger value of u as $x \to +\infty$. An *antikink* is the opposite. Here I give the beginnings of an analysis of the interaction of a widely separated kink and antikink, using my approach (it has been studied before by many authors using other methods, e.g. Ref. 51).

The equations can be expressed in Hamiltonian form by defining $\pi = u_t$, Hamiltonian $H(u, \pi) = \int \frac{1}{2}\pi^2 + \frac{1}{2}u_x^2 + V(u)\ dx$ and symplectic form $\Omega((\dot u, \dot\pi), (u', \pi')) = \int \dot u \pi' - u'\dot\pi\ dx$ for a general pair of variations. For concreteness, take $V(u) = \frac{1}{4}(u^2 - 1)^2$. This has kink and antikink solutions $u(x,t) = \pm \tanh \frac{\gamma}{\sqrt2}(x - vt - x_0)$, with associated momentum field $\pi(x,t) = \mp \frac{\gamma v}{\sqrt2}\mathrm{sech}^2 \frac{\gamma}{\sqrt2}(x - vt - x_0)$, for any $x_0 \in \mathbb{R}, v \in (-1, 1)$, where $\gamma = \frac{1}{\sqrt{1-v^2}}$. Linearising about the equilibria $u = \pm1, \pi = 0$ gives waves with frequencies at least $\sqrt{V''(\pm1)} = \sqrt2$.

It suffices to study the interaction in the centre of mass frame, so let us restrict attention to slow manifolds consisting of pairs of even functions

(u, π). A natural initial guess M_0 at a slow manifold is the set of pairs

$$u(x) = 1 + \tanh \frac{\gamma}{\sqrt{2}}(x - x_0) - \tanh \frac{\gamma}{\sqrt{2}}(x + x_0) \tag{21}$$
$$\pi(x) = -\frac{\gamma v}{\sqrt{2}} \left(\operatorname{sech}^2 \frac{\gamma}{\sqrt{2}}(x - x_0) + \operatorname{sech}^2 \frac{\gamma}{\sqrt{2}}(x + x_0) \right),$$

for $|x_0| \gg 1$, v small. This looks like the superposition of a kink at x_0 with velocity v and an antikink at $-x_0$ with velocity $-v$. To obtain the slow equations of motion on M_0 we compute the restrictions of H and Ω to M_0.

The restriction of H to M_0 has already been computed:[51]

$$H|_{M_0}(x_0, v) = H_0(x_0, v) = \frac{1}{2} m_1(x_0, \gamma) v^2 + V_1(x_0, \gamma) + V_2(x_0, \gamma), \tag{22}$$

where the functions m_1, V_1, V_2 are given in equations (B.8a), (B.5a), (B.5b) respectively, of Ref. 51. The symplectic form, however, does not appear to have been computed before (Ref. 51 obtained equations of motion by assuming $\dot{x}_0 = v$ and using conservation of H_{M_0}). I obtain $\Omega|_{M_0} = S(x_0, v)\ dx_0 \wedge dv$, where $S = \gamma^2 m_1 + \gamma^5 v^2 S_1(x_0, \gamma)$ with S_1 a certain integral decaying exponentially like $e^{-2\sqrt{2}|x_0|}$ as $x_0 \to \pm\infty$. Now $m_1(x_0, \gamma) = \gamma(M + K(x_0, \gamma))$, with[51] $M = \frac{4\sqrt{2}}{3}$ (which is just twice the rest energy of a kink) and K exponentially decaying in x_0. So $S = \gamma^3 M + v^2 S_2(x_0, \gamma)$ with S_2 exponentially decaying in x_0. The leading term suggests that instead of the coordinate v on M_0 it might be better to use $p = \gamma M v$, because then $\Omega|_{M_0} = (1 + p^2 S_3)\ dx_0 \wedge dp$, with S_3 exponentially decaying in x_0, but I'll continue with v. The resulting slow equations are:

$$\dot{x}_0 = \frac{1}{S} \frac{\partial H_0}{\partial v} \tag{23}$$
$$\dot{v} = -\frac{1}{S} \frac{\partial H_0}{\partial x_0}.$$

To leading order in v and $e^{-2\sqrt{2}|x_0|}$, it is sufficient to keep only the leading terms of m_1 and S and to ignore the v dependence of V_1 and V_2 (via γ). Then we obtain the approximate slow dynamics

$$\dot{x}_0 = v \tag{24}$$
$$\dot{v} = -12\sqrt{2}\,\mathrm{sgn}(x_0) e^{-2\sqrt{2}|x_0|}$$

(which says that the kink and antikink attract exponentially). For v small and x_0 large, this is indeed slow compared to the minimum frequency of linearised vibrations about the tails ($\sqrt{2}$). It is also slow compared to the linearised vibrations about a kink (the only addition to the spectrum is a shape mode at frequency $\sqrt{3/2}$), and hence presumably slow compared to the linearised frequencies normal to the slow manifold.

Next one should estimate the error vector field, to see how reliable is Eq. (24). Diogo Pinheiro computed that it is of the same order in $(v, e^{-2\sqrt{2}|x_0|})$ as the slow vector field, so M_0 is almost a first order slow manifold except that there is not a small prefactor. It is possible, however, that the slow dynamics is more accurate than the slow manifold. To investigate this, one could apply one iteration of my method, which would produce a second order slow manifold, and see if it makes a significant difference to the slow vector field, and this is under investigation.

Example 10: Motion of a kink in a lattice

For a spatial discretisation of a nonlinear wave equation with kinks, there are still stationary kinks (generally one centred on a site and one on a bond, with energies differing by the so-called Peierls-Nabarro barrier), but it is believed to be unlikely that there are travelling ones, except perhaps for some isolated speeds (for a recent article on this which includes references to the basic but not yet rigorous intuition, see Ref. 52)[c]. Numerics (e.g. Ref. 54), however, show existence of approximate travelling kinks, which travel as if in a periodic potential, of period equal to the lattice spacing. There should be a slow manifold describing this, so it would be interesting to apply my method. Some discretisations have no Peierls-Nabarro barrier, but still appear not to have true travelling kinks,[55] though there is also a completely integrable discretisation of the sine-Gordon PDE.[56] An interesting change of coordinates to study the motion of kinks in a lattice and their radiation was obtained in Ref. 57. Also the interaction of travelling kinks with impurities in the lattice has been studied.[58] For more sophisticated work on the motion of kinks, in particular the radiation damping effects which place an ultimate limit on the accuracy of a slow manifold, see Ref. 37.

Note that motion near a normally elliptic symplectic slow manifold of a Hamiltonian system can differ substantially from that on the manifold. There can be adiabatic invariants for the normal oscillations which produce substantial net forces on the slow degrees of freedom. For example, for a charged particle in a strong magnetic field, there is a slow manifold

[c]Note that travelling pulses do exist in chains of FPU type for all speeds above the sound speed,[53] but the problem with discretisations of nonlinear wave equations is that for every speed except zero there is a phonon with the same phase speed.

corresponding at lowest order to motion along the field lines at constant speed, but nearby trajectories execute helices around the field lines with adiabatic invariant $\mu = v_\perp^2/2B$, whose instantaneous centre s experiences a force $-\mu\ \partial B/\partial s$ along the field line, leading to mirroring at places where the field is too strong (compared to the ratio of the kinetic energy to μ).

6. The Methods of Collective Coordinates

The method of the previous section bears a resemblance to two traditional methods for constructing slow dynamics, both often called the method of collective coordinates. To clarify the situation, I propose to call them the methods of "coordinate change" and "constrained Lagrangians".

The method of coordinate change consists of constructing a canonical coordinate change for a Hamiltonian system such that some of the new coordinates represent degrees of freedom of coherent structures and the rest represent "radiation". If the coordinates are well chosen, the submanifold corresponding to zero radiation is found to be almost invariant, at least the part of it where the motion is slow. It was proposed by Sakita and collaborators, but formulated most clearly in Ref. 59, became a standard technique in quantum field theory, and has been used occasionally in classical mechanics (e.g. Ref. 60). I am not aware, however, of a systematic procedure for choosing the coordinate change, nor for improving a choice. Also the restriction to canonical coordinate changes makes more work in my opinion than allowing the symplectic form to become nonstandard.

The method of constrained Lagrangians has been widely used in classical mechanics, e.g. Refs 55, 58, 61-65. Here I assess its validity or otherwise, which I have not seen examined adequately before. It is best formulated in the Lagrangian rather than Hamiltonian context.

Lagrangian systems are those that arise from a variational principle of the form $\delta \int L(q, \dot{q})\ dt = 0$ for some function $L : TQ \to \mathbb{R}$ on a tangent bundle TQ (the points of TQ consist of a point q of Q together with a tangent vector v there) satisfying the *Legendre condition* that $v \mapsto p = \frac{\partial L}{\partial v}$ is invertible at each $q \in Q$, giving rise to the *Euler-Lagrange equations* of motion $\dot{\frac{\partial L}{\partial v_i}} = \frac{\partial L}{\partial q_i}, \dot{q}_i = v_i$ in local coordinates q_i on Q. Any Lagrangian system can be converted to an equivalent Hamiltonian system on the cotangent bundle T^*Q (a *cotangent vector* p at $q \in Q$ is a linear map from $T_qQ \to \mathbb{R}$), by defining $H(q, p) = p \cdot v - L(q, v)$, where $v(q, p)$ is defined by the Legendre condition and $p \cdot v$ is the natural pairing of cotangent and tangent vectors, and using the canonical symplectic form $\Omega = -d(p \cdot dq)$ on T^*Q (note that this is my choice of where to put the inescapable minus sign of Hamiltonian mechanics). Similarly any Hamiltonian system on a cotangent bundle with $p \mapsto v = \frac{\partial H}{\partial p}$ invertible at each $q \in Q$ defines an equivalent Lagrangian system with $L(q, v) = p \cdot v - H(q, p)$.

In the method of constrained Lagrangians, one proposes as slow manifold the tangent bundle TQ_0 of a submanifold Q_0 of the configuration space Q and computes equations of motion on it by restricting the variational principle to TQ_0. These are generally assumed to be good approximate slow dynamics for the original system, but I have not seen this assumption justified in general[d]. Indeed there are plenty of choices for Q_0 for which the resulting dynamics has nothing to do with the original dynamics. Even for plausible choices of Q_0, the ansatz may need significant correction, e.g. Ref. 66. In general, to assess the accuracy of the slow manifold, one has to check the difference between the two vector fields. Equivalently, one has to check the size of the constraining force, though this is something that is not directly accessible in Lagrangian dynamics (which is why Lagrange was so proud of his formulation of mechanics: it allows one to compute constrained dynamics with no need to compute the constraining forces). The difference between the two vector fields is determined by dH on tangent vectors in TTQ transverse to TTQ_0, since in the notation of Ref. 68 the vector field Z at $v \in T_qQ$ is determined by $\Omega_L(v)(Z, w) = dH(v) \cdot w \ \forall w \in T_vTQ$ and the vector field Z_0 at $v \in T_qQ_0$ is determined by $\Omega_L(v)(Z_0, w) = dH(v) \cdot w \ \forall w \in T_vTQ_0$.

Any slow manifold TQ_0 for a Lagrangian system can be improved to a first order one TQ_1, as follows. Construct a foliation $\bigcup_{q \in Q_0} F_q$ transverse to Q_0. The normal dynamics being fast compared to the tangential dynamics implies that for each $q \in Q_0$ there is a locally unique critical point $\tilde{q}(q)$ of the restriction of $L(\tilde{q}, 0)$ to F_q. Then $Q_1 = \{\tilde{q}(q) : q \in Q_0\}$ is a smooth submanifold containing all equilibria in a neighbourhood of Q_0 and a straightforward calculation shows the error vector field for the resulting constrained Lagrangian on TQ_1 is relatively small.

A severe disadvantage of the method of constrained Lagrangians is that although TQ_0 can be improved to a first order slow manifold TQ_1, there is no way in general to improve it to a second order slow manifold. The reason

[d]Some cases close to completely integrable can be justified by perturbation theory for completely integrable systems, e.g. Ref. 67, and there are proofs for some other specific systems, e.g. Ref. 26; there are also methods based on "elimination of secular perturbations or unbounded fluctuations",[51] but I do not find the arguments totally convincing.

is that second order slow manifolds of the Hamiltonian context are in general not the cotangent bundle of a submanifold of the configuration space, e.g. q_0 an equilibrium does not imply there is a second order slow manifold containing all small tangent vectors at q_0, as can be seen in the spring pendulum. Indeed there are some problems, e.g. in atmospheric dynamics, where even the natural zeroth order slow manifolds are not cotangent bundles (see next section).

7. Velocity Splitting

Since Ref. 65, there has been quite an industry, e.g. Ref. 29 and references therein, producing symplectic slow manifolds of the special form $p = P(q)$ for Hamiltonian systems of the standard mechanical form $H(q,p) = \frac{1}{2}p^T M^{-1}p + W(q)$ on a cotangent bundle T^*Q, with the canonical symplectic form, by a technique called "velocity splitting" (they take M to be the identity matrix, but I will allow any constant invertible symmetric matrix in my exposition, and I expect one could extend to non-constant M). Here I compare the velocity splitting method with mine.

Their procedure is firstly to imagine that workless constraint forces are introduced to force $p = P(q)$, and to compute the resulting evolution $\dot{q} = U(q)$ of q by the standard theory of constrained Hamiltonian systems (as in the second paragraph of section 5). The result is that

$$U = -\Omega_0^{-1}(\nabla W + DP^T M^{-1} P), \tag{25}$$

where $\Omega_0 = DP - DP^T$ (the matrix representing the restriction of the symplectic form to the submanifold) is assumed invertible (note that this requires the dimension of Q to be even). This is just the condition for $p = P(q)$ to be symplectic, and the resulting dynamics is precisely that I would use on the slow manifold in Section 5 (though my U would also have a p-component $\dot{p} = DP\ U$).

Secondly, they compare U with $M^{-1}P$, proving that they are identical vector fields iff the constraint forces are zero. The difference $U^S = U - M^{-1}P$ is called the *velocity split* (this is just the configuration space component of my $U - V$, but the p-components take care of themselves in this simple context). So a slow manifold with identically zero velocity split is invariant.

Thirdly, some have proposed an iterative scheme to improve the slow manifold to one of a higher order of accuracy, namely to replace the field P by $\tilde{P} = MU$, but I am not aware of any argument for why this should be any better. In fact, it is not any better unless DP happens to satisfy some special conditions.

To see this, consider the step that their iteration takes along the symplectically orthogonal foliation given by affinely extending the symplectically orthogonal subspaces. The symplectically orthogonal subspace at $(q, P(q))$ is $\{(\xi, DP^T\xi) : \xi \in T_qQ\}$. It is convenient to assume DP invertible (as holds at generic points) and write this as $\{(DP^{-T}\eta, \eta) : \eta \in T_q^*Q\}$. In the iterative step the displacement of the slow manifold is vertically by MU^S. To first order, this is equivalent to a displacement along the symplectically orthogonal foliation by

$$\eta = (I - DP\ DP^{-T})M\ U^S = -DP^{-T}\Omega_0 MU^S. \tag{26}$$

Now DH acting on a general symplectically orthogonal vector $(DP^{-T}\eta', \eta')$ is $\nabla W^T DP^{-T}\eta' + P^T M^{-1}\eta'$. So $DH|_F$, when regarded as a vector to be dotted with vertical vectors η', is $DP^{-1}\nabla W + M^{-1}P$. Comparing with (25) shows that $DH|_F = -DP^{-1}\Omega_0 U^S$. My method takes the step along F which makes $DH|_F$ zero. To first order this is the Newton step $-D^2H|_F^{-1}DH|_F(q, P(q))$, and only steps which agree with this to first order give first order accuracy. Now $D^2H|_F = DP^{-1}D^2W\ DP^{-T} + M^{-1}$ with respect to the vertical coordinate η'. So the Newton step is

$$(DP^{-1}D^2W\ DP^{-T} + M^{-1})^{-1}DP^{-1}\Omega_0 U^S. \tag{27}$$

We see that the two steps (26) and (27) are the same for general U^S iff

$$(DP^{-1}D^2W DP^{-T} + M^{-1})DP^{-T}\Omega_0 M = -DP^{-1}\Omega_0. \tag{28}$$

If the submanifold is slow then D^2W should be negligible here, so neglecting it and writing $B = DP^{-1}DP^T$, the condition for equality becomes $B^{-1}M = MB$.

To appreciate what sort of restriction this condition imposes on DP, consider the case where M is a multiple of the identity. Then it says $B^2 = I$, so $B = C^{-1}EC$, where E is any diagonal matrix of ± 1 and C any invertible matrix. It follows that $C\ DP^T = E\ C\ DP$. Partition the coordinates into blocks labelled $+$ and $-$ according to the sign of E on them, and write out the equations for the blocks of C and DP. A simple calculation shows that Ω_0 acting on $[C_{++}^T, C_{+-}^T]$ gives zero, so Ω_0 is degenerate unless the dimension of the $+$ space is zero. But $E = -I$ implies DP is antisymmetric. So if the mass matrix M is a multiple of the identity then the only case when the step of Ref. 29 pushes the error one order higher is when DP happens to be antisymmetric. It seems that it is close to antisymmetric for most of their applications, so their iteration does lead to improvement, but for a fortuitous reason. It would be interesting to examine the consequences of $B^{-1}M = MB$ on DP for general M.

My method has the advantages that it applies to all forms of Hamiltonian system and to all forms of symplectic submanifold and the iteration in one step includes all nearby equilibria in the slow manifold and in r steps obtains r^{th} order relative accuracy for the slow dynamics. It would be interesting to apply my method to some of the systems where velocity splitting has been used.

8. Poisson slow manifolds

In some cases, like 3D atmospheric dynamics, the requirement that the candidate slow manifolds be symplectic is too strong: as pointed out in Ref. 69, for these systems the symplectic form always degenerates somewhere on the slow manifold or even everywhere. Theiss proposed a fix via Dirac's theory of constrained Hamiltonian systems, which selects a unique vector field U satisfying $\Omega(U, \xi) = dH(\xi)$ for all ξ tangent to the manifold, by some additional requirements. This can be usefully reformulated in terms of Poisson dynamics.

A *Poisson system* is a vector field U on a manifold M such that for every F in the algebra $A = C^\infty(M, \mathbb{R})$, $dF\ U = \{H, F\}$, where H is a particular function in A and $\{\cdot, \cdot\}$ is a Poisson bracket on M, i.e. an antisymmetric bilinear map $A \times A \to A$ satisfying the Jacobi identity $\{J, \{K, L\}\} + \{K, \{L, J\}\} + \{L, \{J, K\}\} = 0$ and Leibniz rule $\{J, KL\} = \{J, K\}L + K\{J, L\}$ for all $J, K, L \in A$. Every Hamiltonian system can be put in Poisson form because to every symplectic form Ω is associated a Poisson bracket $\{F, G\} = \Omega(X_F, X_G)$, where for general function F, X_F denotes the Hamiltonian vector field of (F, Ω), and then $dFX_H = \{H, F\}$.

Given any submanifold M (not necessarily symplectic) one can restrict the Hamiltonian and the Poisson bracket to it (by choosing any transverse foliation and extending functions on M to be constant along the leaves) and obtain a Poisson system on M. If the Poisson bracket is degenerate on M (meaning there exists a nonconstant function C on it such that $\{C, K\} = 0$ for all functions K) then M decomposes into symplectic leaves which are invariant under all Poisson flows on it and on which the Poisson bracket is non-degenerate and so the flow on the leaves is Hamiltonian.

9. Slow manifolds!with Internal Oscillation

In Hamiltonian systems, there are often submanifolds consisting of approximate periodic orbits, and one wishes to know to what extent there is an invariant manifold nearby on which the motion is approximately periodic on order-one times but with a slow drift to be determined. I call such a manifold a *slow manifold with internal oscillation*.

A couple of examples where this situation arises are the interaction of discrete breathers with frequencies close to rational ratio, and the interaction of Q-balls.

Example 11: Interaction of discrete breathers

Discrete breathers (DB) are time-periodic spatially localised motions of dynamical networks of units. Ref. 6 addressed the question of what happens if one takes as initial condition something close to a superposition of two (or more) widely separated discrete breathers of close frequencies (or more generally, frequencies close to a low order rational ratio). How do their relative phases evolve? Do they exchange energy? For Hamiltonian systems of the form $H(q,p) = \sum_j H_j(q_j,p_j) + \varepsilon H'(q,p)$ with ε small, the H_j nonisochronous and suitable coupling H', we showed that there is an almost invariant symplectic slow manifold consisting of states which look like superpositions of such discrete breathers, and an effective Hamiltonian on it, such that the true evolution is close to that of the effective Hamiltonian. More results on these questions will be presented in Examples 13 and 14 for the special case of "discrete self trapping systems" and in Examples 15 and 16 for general Hamiltonian networks.

Example 12: Interaction of Q-balls

Q-balls are solutions of the form

$$u(x,t) = e^{\mathrm{i}\omega t} f_\omega(r) \tag{29}$$

with ω, f real, $f'(0) = 0$, and $f(r) \to 0$ as $r \to \infty$, where $r = |x|$ relative to some origin, for complex nonlinear field equations

$$u_{tt} = \Delta u - u\beta(|u|^2), u(x,t) \in \mathbb{C}, x \in \mathbb{R}^N, \tag{30}$$

where Δ is the Laplacian and β real. By Poincaré invariance of the field equation, the above stationary Q-balls can be Lorenz boosted to obtain moving Q-balls. To demonstrate the Hamiltonian structure of the field equation, introduce the momentum field $\pi = u_t$, the Hamiltonian $H(u,\pi) = \int \frac{1}{2}(|\pi|^2 + |\nabla u|^2) + V(|u|^2)\ d^N x$, where $V(z) = \int_0^z \beta(s)\ ds$, and symplectic form $\Omega((\dot{u},\dot{\pi}),(u',\pi')) = \int \Re(\bar{\dot{u}} \cdot \pi' - \bar{u}' \cdot \dot{\pi})\ d^N x$. A nice exposition is given in the introduction to Ref. 28 (including how to evaluate the functional derivatives of H). Ref. 70 investigated the question of what happens if two Q-balls of close frequency are fired at each other. The authors found numerically that they attract if the relative phase is 0, repel if the relative phase is π, and exchange "charge" if the relative phase is in between. The method of the next section can be expected to supply an effective Hamiltonian to explain these results.

The case of Hamiltonian systems for which an open subset (rather than a proper submanifold) of the state space consists of approximate periodic orbits was treated by Poincaré,[71] Chirikov[72] and Moser,[73] who obtained slow equations of motion for the parameters of the periodic orbits (in Poincaré's case this was the slow evolution of the parameters of the instantaneous Kepler ellipses for the planets). A recently studied system of this type is described in Ref. 74 and it would be interesting to apply the Poincaré-Chirikov-Moser method to it. Such situations are not the point of my lecture-notes, however; rather I am addressing how to obtain proper submanifolds with slow dynamics (modulo internal oscillation).

In Ref. 6 we treated a case when a proper submanifold consists of approximate periodic orbits and the normal motion is fast compared to the drift between periodic orbits. In the next two sections I give a better treatment, which has the advantage that it can be iterated to arbitrary order of accuracy.

Slow manifolds with internal oscillation can also arise for general (as opposed to Hamiltonian) dynamical systems. In particular, if a slow manifold with internal oscillation is normally hyperbolic then there exists an invariant slow manifold nearby, because internal oscillation implies that any tangential contraction or expansion is at a subexponential rate.

A generalisation which I will not treat in detail here, is to slow manifolds with more internal dynamics than one oscillation, for example quasiperiodic or chaotic. One approach to this is to extend the loop dynamics of Section 11 to the dynamics of other embedded manifolds (cf. Kuksin, private communication), to which similar symmetry reduction can be applied. Averaging with respect to quasiperiodic dynamics is in general much more delicate than for periodic dynamics, e.g. Refs 2, 35, 40, because the quasiperiodic frequency vector can come close to low order commensurability, thereby generating additional slow directions. Averaging with respect to chaotic dynamics can lead to non-Hamiltonian stochastic effective dynamics for the slow variables (I'll write something on this in Ref. 75).

10. Internal oscillation: $U(1)$-symmetric Hamiltonians

Slow manifolds with internal oscillation (other than normally hyperbolic ones) are most easily treated in the special case of Hamiltonian systems with a $U(1)$ symmetry, e.g. the complex field for Q-balls above and discrete self-trapping systems to be introduced below. Note that symmetry of a Hamiltonian system means both the Hamiltonian and the symplectic form are invariant under an action of the symmetry group.

Example 13: Discrete Self-Trapping Systems (DST)
Discrete self-trapping systems (e.g. Ref. 62) have equations of the form

$$\mathrm{i}\dot{\psi}_s = -\gamma_s|\psi_s|^2\psi_s - \sum_{r\in S} C_{sr}\psi_r, \tag{31}$$

where s ranges over a discrete space S, each $\psi_s \in \mathbb{C}$, $\gamma_s \in \mathbb{R}$ and C is real symmetric. Note that for C diagonal, one obtains decoupled units with solution $\psi_s(t) = Ae^{\mathrm{i}\omega_s(|A|^2)t}$, for any $A \in \mathbb{C}$, with the frequency function

$$\omega_s(n) = C_{ss} + \gamma_s n. \tag{32}$$

A special case of the DST is the discrete nonlinear Schrödinger equation (DNLS), where $S = \mathbb{Z}$ and $C_{rs} = C_{00}$ for $r = s$, C_{10} for $|r - s| = 1$ and 0 otherwise (one can also generalise the DST to allow complex Hermitian C and nonlinear terms of the form $\beta_s(|\psi_s|^2)\psi_s$ for real functions β_s, and to other forms of coupling, e.g. the Ablowitz-Ladik equation[62]).

The DST have a Hamiltonian formulation with Hamiltonian

$$H = -\frac{1}{4}\sum_s \gamma_s|\psi_s|^4 - \frac{1}{2}\sum_{r,s} C_{rs}\bar{\psi}_r\psi_s, \tag{33}$$

and symplectic form $\Omega = \frac{\mathrm{i}}{2}\sum_s d\psi_s \wedge d\bar{\psi}_s$, i.e.

$$\Omega(\dot{\psi}, \psi') = \Im(\sum_s \bar{\dot{\psi}}_s\psi'_s). \tag{34}$$

Note that in computing the equations of motion from this formulation, ψ_s and $\bar{\psi}_s$ are to be thought of as independent variables (equivalent to two linear combinations of the real and imaginary parts). The DST have the $U(1)$ symmetry $\psi \mapsto e^{\mathrm{i}\theta}\psi$ for all $\theta \in S^1$.

They have many discrete breathers of the special form $\psi_s(t) = e^{\mathrm{i}\omega t}\phi_s$, ω real (i.e. $U(1)$ orbits), where ϕ is a spatially localised solution of an associated ω-dependent real static problem. The (signed) quantity ω is called the *frequency* of the $U(1)$-symmetric DB.

For a Hamiltonian system with a $U(1)$ symmetry, by Noether's theorem (e.g. Ref. 68) there is an associated conserved quantity A. For (30) it is the *charge* $Q = \int \Im(\bar{u}\pi)\ d^N x$. For DST it is the *number* $N = \sum_s |\psi_s|^2$ (called "norm" by Ref. 62, but it is not of degree 1 so is not a norm though its square is; the term "number" refers to the integer number of quanta in the quantum mechanical case, but classically it can be any non-negative real). In this case, one can reduce the study of the dynamics to that on the quotient spaces P_a, with $a \in \mathbb{R}$, i.e. the $U(1)$-equivalence classes with $A = a$. The Hamiltonian and symplectic form on P_a are just those induced by the original problem. If the internal oscillation corresponds to $U(1)$-orbits, then this reduction turns the problem of a slow manifold with internal oscillation into a standard slow manifold problem, because the periodic orbits are mapped to equilibria of the reduced system. For any order r of accuracy, one obtains a one-parameter family of *effective Hamiltonians* H_a for the reduced system by the method of Section 5.

Example 14: Targeted energy transfer (TET) in a DST

The setting[76] is a DST for which the coupling (off-diagonal part of C) is weak and there is an $a > 0$ and two units i, j with frequency functions such that $\omega_i(n), \omega_j(a-n)$ are (i) close for all $n \in [0, a]$, and (ii) far from the set $F = \{C_{ss} : s \in S \setminus \{i, j\}\}$ of linearised frequencies about the other units (note that in contrast to the next section, there is no need here to require $k\omega$ to avoid F for more $k \in \mathbb{Z}$ than $k = 1$). Then let H_a be the restriction of H to the $U(1)$-equivalence classes of configurations ψ with $N(\psi) = a$ (I'll write the equivalence relation as $\psi \sim e^{\mathrm{i}\theta}\psi$ for all $\theta \in S^1$), and Ω_a the associated symplectic form. Let M_0 be the set of $U(1)$-equivalence classes of superpositions $\psi = e^{\mathrm{i}\theta_i}\sqrt{n}\ \delta_i + e^{\mathrm{i}\theta_j}\sqrt{a-n}\ \delta_j$ with $\theta_i, \theta_j \in S^1, n \in [0, a]$, where for general $k \in S$, δ_k is the configuration with value 1 on unit k and 0 elsewhere. Topologically, M_0 is a 2-sphere, because it is diffeomorphic to the complex projective space $\mathbb{C}P^1$. For coordinates on the sphere I'll use height $n \in [0, a]$ and longitude $\theta = \theta_j - \theta_i$, though of course this coordinate system has a singularity at the poles $n = 0, a$. It is a symplectic submanifold, with Ω_{M_0} the standard area on the 2-sphere ($d\theta \wedge dn$).

For zero coupling, M_0 is an invariant manifold for H_a. The motion on the sphere is a differential rotation about the polar axis at rate

$$\omega_d(n) = \omega_j(a-n) - \omega_i(n), \tag{35}$$

which by assumption (i) is slow. The poles are equilibria, representing all the excitation being on unit i or j, respectively. The normal motion is oscillation at frequencies $C_{ss} - \bar{\omega}(n), s \in S \setminus \{i, j\}$, where $\bar{\omega}(n)$ depends on choice of trivialisation of the normal bundle around the orbit but can be taken to be close to $\omega_i(n)$ for $n \geq a/2$ and to $\omega_j(a-n)$ for $n < a/2$ (the normal bundle to this $\mathbb{C}P^1$ in $\mathbb{C}P^N$ is an example of a non-trivialisable bundle, having first Chern number $c_1 = 1$, e.g. Ref. 77, so there is no natural choice). Thus by assumption (ii), the normal motion is fast. So M_0 is an invariant symplectic slow manifold for no coupling.

For small coupling, M_0 is still a symplectic slow manifold, though not in general invariant. Let us compute the constrained motion on it. We have

$$\begin{aligned} H_{M_0} = &-\frac{1}{2}(\gamma_i n^2 + \gamma_j (a-n)^2) \\ &-C_{ii} n - C_{jj}(a-n) - 2C_{ij}\cos\theta\sqrt{n(a-n)}, \end{aligned} \tag{36}$$

and $\Omega_{M_0} = d\theta \wedge dn$, so

$$\begin{aligned} \dot\theta &= \omega_d(n) - \frac{a-2n}{\sqrt{n(a-n)}} C_{ij}\cos\theta \\ \dot n &= 2C_{ij}\sqrt{n(a-n)}\sin\theta. \end{aligned} \tag{37}$$

Note that if $C_{ij} \neq 0$ the equilibria move away from the poles (to see this it is best to change to coordinates $x = \sqrt{n(a-n)}\cos\theta, y = \sqrt{n(a-n)}\sin\theta$). The resulting dynamics may not be meaningful, however, as the errors can be of similar order if C_{ij} (or $\varepsilon^{d(i,j)}$ in the case of nearest neighbour coupling ε) is comparable to $\omega_d(n)$. So let's apply the procedure of Section 5 to obtain a better slow manifold M_1.

For foliation choose the leaves $F_{\theta,n}$ to be the set of $U(1)$-equivalence classes of $\psi = e^{\mathrm{i}\theta_i}\sqrt{(1-\eta)n}\ \delta_i + e^{\mathrm{i}\theta_j}\sqrt{(1-\eta)(a-n)}\ \delta_j + \tilde\psi$ such that $\theta_j - \theta_i = \theta, \tilde\psi_i = \tilde\psi_j = 0$, and $\eta = N(\tilde\psi)/a$. Then we seek the unique critical point of H_a on $F_{\theta,n}$ with η small. Differentiating with respect to $\bar\psi_s, s \in S \setminus \{i,j\}$, the equations for the critical point are:

$$\begin{aligned} &\frac{G}{a}\tilde\psi_s - \gamma_s|\tilde\psi_s|^2\tilde\psi_s - \sum_{r\notin\{i,j\}} C_{sr}\tilde\psi_r \\ &\quad = C_{si}e^{\mathrm{i}\theta_i}\sqrt{(1-\eta)n} + C_{sj}e^{\mathrm{i}\theta_j}\sqrt{(1-\eta)(a-n)}, \end{aligned} \tag{38}$$

where

$$\begin{aligned} G = \ &\gamma_i(1-\eta)n^2 + C_{ii}n + \gamma_j(1-\eta)(a-n)^2 + C_{jj}(a-n) \\ &+2C_{ij}\sqrt{n(a-n)}\cos\theta + \textstyle\sum_{r\notin\{i,j\}} C_{ir}\Re(e^{-\mathrm{i}\theta_i}\tilde\psi_r)\sqrt{\frac{n}{1-\eta}} \\ &+ \textstyle\sum_{r\notin\{i,j\}} C_{jr}\Re(e^{-\mathrm{i}\theta_j}\tilde\psi_r)\sqrt{\frac{a-n}{1-\eta}}. \end{aligned} \tag{39}$$

To first order in $\{C_{si}, C_{sj} : s \in S \setminus \{i,j\}\}$, $\tilde{\psi}$ is given by the solution of the affine system

$$\frac{G_0}{a}\tilde{\psi}_s - \sum_r C_{sr}\tilde{\psi}_r = C_{si}e^{\mathrm{i}\theta_i}\sqrt{n} + C_{sj}e^{\mathrm{i}\theta_j}\sqrt{a-n}, \tag{40}$$

where $G_0 = \gamma_i n^2 + C_{ii} n + \gamma_j (a-n)^2 + C_{jj}(a-n) + 2C_{ij}\sqrt{n(a-n)}\cos\theta$ and $\eta = 0$. To obtain a first order slow manifold one should solve (39) and $N(\tilde{\psi}) = a\eta$ exactly for $\tilde{\psi}(\theta, n; a)$, and substitute the result into (33) and (34) to obtain some $H_{M_1}(\theta, n; a)$ and $\Omega_{M_1}(\theta, n; a) = \phi(\theta, n; a)\ d\theta \wedge dn$ for some function ϕ. Then the slow dynamics on M_1 is given by

$$\begin{aligned} \dot{\theta} &= \frac{1}{\phi}\frac{\partial H_{M_1}}{\partial n} \\ \dot{n} &= -\frac{1}{\phi}\frac{\partial H_{M_1}}{\partial \theta}. \end{aligned} \tag{41}$$

Many different phase portraits can occur, depending on the frequency difference function ω_d and the coupling. See Fig. 3 for some sketches. Parts (a-e) and (f-i) of the figure are sequences as the coupling is increased from zero for systems where ω_d has one sign change and no sign changes, respectively. For comparison, parts (j-m) of the figure show the case of two coupled oscillators with interchange symmetry, familiar from modelling of vibrations of water and other symmetric triatomic molecules, progressing from small to large amplitude at fixed coupling.

Because the slow dynamics is Hamiltonian and on a 2-sphere, all orbits are periodic except equilibria and separatrices (orbits asymptotic to equilibria). In particular, as a codimension-1 phenomenon achievable in some examples by suitable choice of total number a, there can be a periodic trajectory from one pole to the other and back, in which case the energy exchanges completely and periodically between the configurations they represent. A necessary and sufficient condition for this is that the poles have the same value of H_M, not be equilibria, and there be no separatrix dividing them (Ref. 76 neglects to mention the last condition). Limiting cases of codimension 3 and 5 are that one pole is a saddle and the other lies on a separatrix from it, or both poles are saddles and are connected by a separatrix.

Extensions of the TET theme have been proposed by Aubry, e.g. a transistor and an AND gate using discrete breathers, creating the concept of “breathonics”.

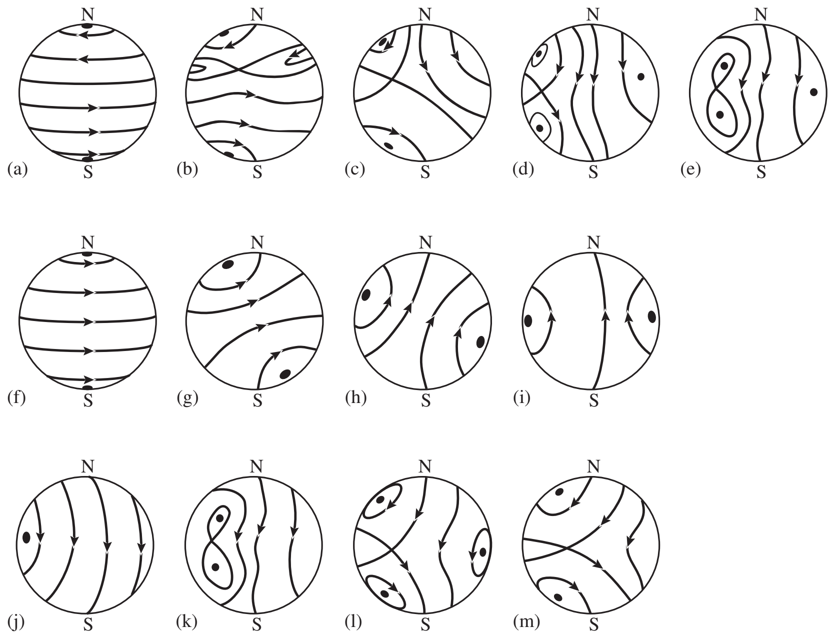

Fig. 3. Three series of examples of phase portraits for the effective Hamiltonian on a sphere: (a) uncoupled oscillators with one sign change in ω_d, (b) effect of generic weak coupling, (c) a possible effect of larger coupling, (d) yet larger coupling, (e) complete energy transfer; (f) an uncoupled case with no sign change, (g) effect of generic weak coupling, (h) a possible effect of larger coupling, (i) complete energy transfer; (j) a $\mathbb{Z}_2$-symmetric system in the linear regime (note that it exhibits complete energy transfer at a frequency proportional to the coupling, and the equilibria represent the symmetric and antisymmetric normal modes), (k) sufficient nonlinearity causes one of the normal modes to lose stability and create a pair of asymmetric equilibria, (l) greater nonlinearity makes the asymmetric equilibria take on a more local character, (m) yet greater nonlinearity stops the energy transfer.

One can also apply the method to DST systems with given coupling and two families of $U(1)$ discrete breathers $D_1(n)$, $D_2(n)$, assumed already known, parametrised by their number n, with frequencies $\omega_1(n)$ and $\omega_2(a-n)$ close for some choice of a, and non-degenerate equilibria of the reduced Hamiltonians H_n and H_{a-n} respectively; note that non-degeneracy requires conditions on both the phonon spectrum for the zero state and the frequencies of any shape modes[e] of the breathers. One makes a

[e] *Shape modes* on a spatially localised solution are oscillatory solutions of the linearised equations about it which are themselves spatially localised: for a $U(1)$ discrete breather

slow manifold by a superposition of the breathers with given total number: $M_0 = \{\psi = (e^{i\theta_1} D_1(n_1) + e^{i\theta_2} D_2(n_2))_\sim : N(\psi) = a, n_1, n_2 \geq 0, \theta_1, \theta_2 \in S^1\}$. It is again diffeomorphic to $\mathbb{C}P^1$ and the poles are equilibria, representing $D_1(a)$ and $D_2(a)$. One can then apply the method of Section 5 to construct a higher order slow manifold, but note that it will continue to include the exact discrete breathers $D_1(a)$ and $D_2(a)$ as equilibria at the poles, because they are present by assumption, so there is no energy transfer between them, except for the codimension-1 possibility that they are both saddles at the same energy and possess a separatrix joining them. There may, however, be energy transfer from near $D_1(a)$ to near $D_2(a)$.

As a second example, the method can be applied to compute the interaction of two widely separated Q-balls of close frequency: the effective dynamics is on a space of relative separation, relative velocity (or momentum), phase difference and frequency (or charge) difference, which has dimension $2N + 2$ for N space dimensions. This will be reported in a forthcoming paper.

One question for slow manifolds with $U(1)$ symmetry is to what accuracy one can recover the rate of change of phase of the internal oscillation. An immediate problem is to decide how the phase above one point of the reduced space is related to that above nearby points. One way is via the Hannay-Berry connection,[79] but note that in general it has non-trivial holonomy, i.e. following locally constant phase round a loop on the reduced space one may find one returns to a different phase from the initial one, the phase change being given by the integral of a certain 1-form around the loop. With this choice, I would expect the rate of change of the phase to be order r close to $\frac{\partial H_a}{\partial a}$, which is the instantaneous frequency. It would be interesting to prove (or disprove) this.

11. Internal oscillation: General Hamiltonians

Although $\mathbb{T}^d$ symmetry (and hence many $U(1)$ subgroups) arises to arbitrarily high order near a generic elliptic equilibrium point in a Hamiltonian system of d degrees of freedom (Birkhoff normal form), existence of an exact $U(1)$ symmetry is a special situation. Also the treatment of the previous section does not apply to internal oscillations of $U(1)$-symmetric systems if they are not $U(1)$ orbits. So it is important to generalise the method of the previous section. A first step in this direction was made in Ref. 6,

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the question of existence of shape modes reduces to linearisation about an equilibrium, for which there are good methods, e.g. Ref. 78.

but there we could not see how to make iterative improvements beyond the first, which is rectified here.

The idea is to turn the problem of slow manifolds with internal oscillation into a standard slow manifold problem for *loop dynamics*, i.e. the induced dynamics on the loop space $\tilde{P} = \{z : \mathbb{R}/\mathbb{Z} \to P\}$, where each point of a loop evolves independently of the others, according to Hamilton's equations. This can be written[80] as a Hamiltonian system on $\tilde{P}$, by choosing $\tilde{H}(z) = \oint H(z(s))\ ds$ and $\tilde{\Omega}(\zeta, \xi) = \oint \Omega(\zeta(s), \xi(s))\ ds$. Now loop dynamics has a $U(1)$ symmetry: $(R_\theta z)(s) = z(s + \theta), \theta \in \mathbb{R}/\mathbb{Z}$. The associated conserved quantity is the *area* $A(z) = \int_{D_z} \Omega$ (often $A/2\pi$ is called "action", but this word is used for so many different things that I prefer to avoid it), where D_z is any disc spanning the loop z (the value of $A(z)$ might depend on the homotopy class of D_z but it does not vary under continuous deformation of D_z fixing the boundary z). So we can reduce loop dynamics to a Hamiltonian dynamics on $\tilde{P}_a = \{z/U(1) : A(z) = a\}$ and apply the Hamiltonian slow manifold theory of Section 5. A slow manifold in $\tilde{P}_a$ gives an approximately invariant manifold in P consisting of approximate periodic orbits of area a, evolving by an effective Hamiltonian.

To carry out this programme, one first needs to establish what it means for the normal dynamics to be fast in $\tilde{P}_a$. The answer is the *non-resonance condition* that the normal Floquet multipliers of the given periodic orbit should avoid $+1$. This is equivalent to all integer multiples of its frequency avoiding both the phonon spectrum and the frequencies of any shape modes. The non-resonance condition is encountered on trying to make $\tilde{H}_a$ critical on the leaves of a symplectically orthogonal foliation, e.g. representing loops by Fourier series, one needs the variation of $\tilde{H}$ with respect to all Fourier coefficients (except those representing tangents to the slow manifold) to be non-degenerate.

Examples to which this method can be applied include generalised multibreathers, targeted energy transfer in general Hamiltonian networks, and travelling discrete breathers, all of which were sketched in Ref. 6. Some examples of travelling discrete breather were treated from this improved point of view in Ref. 81. In particular, the phenomena of Fig. 3 can be expected in general Hamiltonian networks, not just DST.

Example 15: Existence of multibreathers

One of the by-products of the method of this section is existence for Hamiltonian networks of at least n families (parametrised by area) of true periodic orbits (and 2^{n-1} if all are non-degenerate) near superpositions of

n spatially separated near-resonant (i.e. frequencies in rational ratio) DBs with all amplitudes nonzero and satisfying a generic condition (to be given below), called *multibreathers* (Ref. 6 treated the particular case of DBs in a weakly coupled network). The idea is that by applying one iteration of my method, there is a first order symplectic slow manifold (with internal oscillation) consisting of loops that look like superpositions of the n DB with all possible choices of total area a, relative phases θ_i and their rates of change p_i. Thus the reduced slow manifold for given area is diffeomorphic to $\mathbb{T}^{n-1} \times I^{n-1}$, I being an interval. Since the DB are spatially separated, the effective Hamiltonian H_a has small first derivative in p. Next, I formulate the required generic condition on the DB (which we neglected to do in Ref. 6). Denote the energy of the i^{th} DB as a function of its area a by $E_i(a)$. Then its frequency is $\omega_i = E_i'(a)$ (note that the frequency is signed). Let $\beta_i = \omega'(a)$. We are supposing the frequencies to be in close to rational ratio, say $\omega \propto k \in \mathbb{Z}^n$. Then the condition is that $\sum_i (k_i \prod_{j \neq i} \beta_j) \neq 0$. Under this condition, the effective Hamiltonian H_a has invertible second derivative in p. Thus for each θ there is a locally unique $p(\theta)$ such that the first derivative is zero. These points form a smooth submanifold diffeomorphic to $\mathbb{T}^{n-1}$. Let $V(\theta) = H_a(\theta, p(\theta))$. Then V is a smooth function on an $(n-1)$-torus so by Liusternik-Shnirelman theory (e.g. Ref. 77) it has at least n critical points, and by Morse theory if all its critical points are non-degenerate there are at least 2^{n-1}. Critical points of V correspond to true periodic orbits, giving the multibreathers. If the method is carried to second order then one obtains the exact slow part of the linearised dynamics about the periodic orbits (in contrast to Ref. 6 where we were able to obtain only approximate linearised dynamics).

Example 16: Travelling discrete breathers

The method allows one to identify parameter regimes for Hamiltonian systems on periodic lattices where DB should travel well,[81] and puts the concept of Peierls-Nabarro barrier for DB on a firm footing (extending the proposal of Ref. 82 from the $U(1)$-symmetric to the general case). The idea is that if there is a slow manifold with internal oscillation of at least first order, containing a DB and its translate by one lattice vector for some value(s) of area a, and the slow dynamics has an orbit which passes from a point close to the DB to its translate by the lattice vector, then that orbit represents a periodically travelling DB, so the original system has a solution which looks approximately like a travelling DB for a long time. The accuracy is better the slower the motion on the orbit (because the slow manifold is at least first order).

In the case of a 2D slow manifold, existence of such an orbit is a consequence of conservation of the effective Hamiltonian, provided the "torsion" (to be defined below) is non-zero; and the maximum speed along the orbit can be quantified roughly by the following concept of barrier to motion of the DB (which is defined for any dimension of slow manifold). Choose coordinates q on the slow manifold to represent the position of the DB. The derivative of the effective Hamiltonian H_a at constant q is small. Assume that the torsion β, i.e. the second derivative of H_a at constant q, is invertible. Then there is a locally unique critical point $z(q, a)$ with respect to variations with constant q and a. Let $V_a(q) = H_a(z(q, a))$. For curves γ connecting the DB to its translate at constant a let $b(\gamma)$ be the variation of H_a on the curve (its maximum minus its minimum). Define the *barrier* $B(a)$ to be the minimum of $b(\gamma)$ over such curves. Note that the given DB is a critical point of V_a and curves minimising b must pass through at least one other critical point, which will also be a DB, so $B(a)$ is given by the difference in energy of some pair of DBs. Then there are orbits of the desired type with maximum speed approximately $\sqrt{B(a)/\beta}$.

An interesting question is what significance the barrier has if the slow manifold is more than two-dimensional (probably not much if the torsion β is indefinite). The same question can be posed for the simpler case of travelling dislocations in more than 1D (where the analogue of the torsion is the kinetic energy, so usually positive definite).

Note that we do not expect exact travelling DB in general (article in preparation), but there can occur[83] exact "nanopterons", i.e. travelling solutions asymptotic to small amplitude phonons at large distance.

Another example to which it would be interesting to apply the method is the interaction of two gyrating charged particles in a 3D magnetic field. One might ask whether the method could be applied to study the interaction of kinks with shape modes, as is required to understand the phenomena reported in Ref. 51 for example. Unfortunately, in a spatial continuum like that of Ref. 51, the phonon spectrum is unbounded, so it is impossible to satisfy the non-resonance condition. The resonance effects are weak for small amplitude of the shape modes, however, so it might nevertheless be possible to construct useful approximate slow manifolds including them. Ref. 37 reports some work in such a direction, including the effects of weak spatial discretisation and estimating the radiative losses.

Note that for $U(1)$-symmetric systems, the methods of this and the previous section can be combined to treat 2-frequency quasiperiodic internal oscillations, provided one of the frequencies corresponds to $U(1)$ orbits. First quotient out the $U(1)$ symmetry as in the previous section, and then consider loop dynamics as in this section, on the reduced space (alternatively, one can consider loop dynamics on the full space and then quotient by the action of $\mathbb{T}^2$ generated by the $U(1)$ symmetry and the phase-shift along loops).

12. Bounds on time evolution

The concern of many authors in the theory and application of slow manifolds is to know for how long true solutions remain close to the solutions of the approximate dynamics, or at least to the slow manifold. There are four main ways of obtaining estimates on these.

The first is *Gronwall estimates*. The idea here is to choose a norm and then use the simple fact that $\dot{e} = f(e,t)$, representing the evolution of the error $e(t)$, with $|e(0)| \leq \eta$, $|f(0,t)| \leq \delta$ and $||\frac{\partial f}{\partial e}|| \leq M$ for $|e| \leq E$, some $E \geq \eta$, implies that $|\dot{e}| \leq \delta + M|e|$. Gronwall's lemma says that it follows that $|e(t)| \leq (\eta + \frac{\delta}{M})e^{Mt} - \frac{\delta}{M}$ as long as the right hand side does not exceed E (this might look a trivial result but the difficulty is that $|e(t)|$ is not necessarily a differentiable function of t). So the error remains at most E as long as

$$t \leq \frac{1}{M} \log \frac{EM + \delta}{\eta M + \delta}. \tag{42}$$

One can do much better than Gronwall estimates, however, if the motion near the given orbit is oscillatory or contracting, because the bound $||\frac{\partial f}{\partial e}|| \leq M$ does not make any distinction between these and the expanding case. Such an improvement is crucial for slow manifolds with oscillatory or contracting normal dynamics because M is of necessity large on the slow timescale and hence the Gronwall estimate (42) is short. One way to obtain improvement is, rather than just a norm, to use a suitable inner product $\langle \cdot, \cdot \rangle$. This is the second method (e.g. Ref. 84). Then $\dot{e} = f(e,t)$ implies

$$\frac{d}{dt}||e||^2 = 2\langle e, f(e,t)\rangle = 2\langle e, f(0,t) + \int_0^1 \frac{\partial f}{\partial e}(\lambda e, t) e \; d\lambda \rangle \leq 2\delta ||e|| + 2\mu ||e||^2, \tag{43}$$

where μ is an upper bound on the spectrum of the symmetric part (with respect to $\langle \cdot, \cdot \rangle$) of $\int_0^1 \frac{\partial f}{\partial e}(\lambda e, t) \; d\lambda$ (which in contrast to the norm can be zero or negative). It follows that

$$||e(t)|| \leq \begin{cases} (\eta + \frac{\delta}{\mu})e^{\mu t} - \frac{\delta}{\mu}, & \mu > 0 \\ \eta + \delta t, & \mu = 0 \\ \frac{\delta}{|\mu|} + (\eta - \frac{\delta}{|\mu|})e^{\mu t}, & \mu < 0 \end{cases} \tag{44}$$

In particular, if $\mu < 0$ then the solution remains within $\frac{\delta}{|\mu|}$ if it starts so. One can often improve the bounds further by choosing an "adapted" inner product (cf. Ref. 85 for the case of a DB of a dissipative network): in the oscillatory case this means one which is chosen to make oscillatory motion round rather than elliptical. Note, however, that in general one would have to allow the inner product to depend on position on the slow manifold and this introduces an additional term in the expression for $\frac{d}{dt}||e(t)||^2$. One can apply the result to the total error or just to the normal component. In the latter case, one can subsequently bound the tangential error in terms of the tangential derivative using the same method.

The above procedure applied to the normal component of the error is a special case of the third method, called the *energy method*. It applies to systems for which there is an "energy" function $E : P \to \mathbb{R}$ (the Hamiltonian is the natural one for many Hamiltonian systems) such that the set $E_<(K) = \{z \in P : E(z) \leq K\}$ is (or at least has as a connected component) a small neighbourhood of the slow manifold for suitable K, and $\frac{dE}{dt}$ is bounded above by some function of position in P. The nicest case is $\frac{dE}{dt} \leq f(E)$ with f Lipschitz. Then $E(t) \leq E_m(t)$, the solution of $\dot{E} = f(E)$ with given $E(0)$, and hence $z(t) \in E_<(E_m(t))$. Once the normal deviation is controlled by this bound, tangential errors can be controlled by Gronwall estimates on the tangential dynamics. For examples of this method, see Refs 4, 2, 7, 28.

The fourth method[49] is *Nekhoroshev estimates*. This applies only to Hamiltonian systems, locally near integrable. By the use of normal form transformations the dynamics in a neighbourhood can be put in a form where the rate of change of half the variables is of arbitrary order in the deviation from integrable in a large fraction of the neighbourhood, and hence the deviation from the orbits on the slow manifold can be bounded as a function of time. In the two degree of freedom case, the deviation can often be bounded for all time because the slow manifold generically has an invariant neighbourhood bounded by KAM tori; the size of the smallest such neighbourhood can be estimated. This method has been used to bound the rate of possible instability of DB [86] and KAM tori,[87] and certain Hamiltonian slow manifolds.[88]

13. Weak Damping

One question that some authors raise about slow-fast systems with oscillatory fast motion is why the observed motion is nearly devoid of fast oscillations even though the models are Hamiltonian (e.g. Ref. 89). I propose the answer is *damping*. A relatively weak amount of damping of the fast oscillations can cause them to die out on a timescale short or comparable to the slow timescale and to be only very weakly excited by the slow motion; bounds to prove this can be obtained by constructing a high order slow manifold and using the inner product method of the previous section, provided it is adapted carefully to the normal oscillations. An illustration of this effect is given in Ref. 33, where numerical damping is found to cause solutions of a Hamiltonian system to converge close to a slow manifold.

Thus in the presence of damping, one can expect to obtain an attracting invariant set with slow motion on it, but it is not necessarily a submanifold (this expectation is shared by the authors of Ref. 90, who propose to call it a "slow quasimanifold"), because candidate submanifolds may contain orbits with stronger tangential contraction than normal contraction, and so the result of Ref. 30 implies generic non-existence of an invariant submanifold. I expect the situation to be closely analogous to that for *Birkhoff attractors*[91] (see also Refs 92, 93). These arise on applying small damping to an area-preserving twist map of an annulus (equivalently, to a typical two degree of freedom Hamiltonian system). If the unperturbed system has a "zone of instability" (meaning a minimal invariant subannulus homotopic to the full annulus) which is mapped into itself by the perturbed map then for large damping the maximal invariant set in the zone of instability is diffeomorphic to a circle, but for weak damping it is an "indecomposable continuum" (a continuum is a compact connected set and it is indecomposable if it can not be written as a (non-disjoint) union of two proper subcontinua). In particular, it is not a circle, and is quite complicated. There is an extensive theory of such invariant sets, and I think it is ripe for exploitation in application areas such as those discussed here (for an introduction and application to a different area, see Ref. 94).

Acknowledgements

My interest in this topic was stimulated by Michael McIntyre and the Newton Institute session on "Mathematics of atmosphere and ocean dynamics", July – Dec 1996; the ideas of Sections 2–4 were developed during that time. In parallel, I had become convinced that in Hamiltonian systems there should be some approximate dynamics associated with the "effective potential" that I'd derived to prove existence of multibreathers,[95] a conviction which initiated the work[6] with Ahn and Sepulchre, so starting off Section 9 and (in a backwards move) the simpler case of Section 5. Shortly afterwards, Richard Battye stimulated my interest in Q-balls, which led to Section 10. The idea of Section 11, which links Ref. 6 with the rest of the work and strengthens it greatly, came to me while preparing a talk for the SIAM Conference on Dynamical Systems and Applications in May 2001. The applications to travelling DB were developed in collaboration with Jacques-Alexandre Sepulchre and benefited from funding by the CNRS and the Research and Training Network LOCNET (EC contract HPRN-CT-1999-00163). I had intended to present the principal results of this paper at the conference in June 2001 in honour of Floris Takens (who wrote one of the important early papers[2] on the subject), but I was unable to attend. Nevertheless, I'd like to dedicate it to him. I used a draft version of these notes in my MSc module in Autumn 2002 and I'm grateful to Diogo Pinheiro and David Stern for many comments which led to improvements, and also to Michael McIntyre for comments on the final version. Finally I'd like to thank Elaine Greaves-Coelho for preparing Figures 2 and 3 and Gill Walton for assistance in transforming the manuscript into World Scientific style.

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