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Collective Induced Phenomena in Systems of Coupled Oscillators

The thesis is submitted in partial fulfilment of the requirements for the award of the degree of Doctor of Philosophy of the University of Portsmouth.

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December 11, 2012
Declaration

Whilst registered as a candidate for the above degree, I have not been registered for any other research award. The results and conclusions embodied in this thesis are the work of the named candidate and have not been submitted for any other academic award.

(Colm Mulhern)
December 11, 2012
Publications


Acknowledgements

My time at the University of Portsmouth has proven to be a most enjoyable experience. This is largely due to my supervisory team whose enthusiasm for my work has made it easy for me to make the transition into research. In particular, I would like to thank my principal supervisor Dr Dirk Hennig for his constant support and guidance. Our many discussions and his meticulous nature have been crucial to my progression through doctoral studies. More than that he has become a dear friend and I will forever remember the many great evenings we spent in the pubs of Portsmouth.

The same applies to my second supervisor Dr Andrew Burbanks who has actively been involved in my work from the beginning. Without him, my programming skill might be limited to a calculator and for this I am truly indebted. His ability to quickly gain insight and understanding of new problems will always amaze me.

Life as a PhD student in Portsmouth has been greatly enhanced by the friends that I have made here. In particular, my office colleagues Wan, Derek, and Simon have provided a friendly and supportive working environment. Also, I would like to thank my team mates at Portchester FC for giving me distractions away from work – I only regret that we did not win some silverware together.

Finally, I cannot thank my family enough. My mother Eileen, father Gabriel, brother Paul and sister Eileen (and little G of course!), have been an undiminishing source of support and belief which has endured throughout my studies. And to Jana
for her constant love and support, and for making it is as easy as possible for me to concentrate on my work when I needed to most.

I acknowledge the financial support provided by the Department of Mathematics without which I would not have been able to undertake a PhD. Further, I would like to thank the head of the Department of Mathematics Professor Andrew Osbaldestin for making it possible for me to attend conferences and workshops.
Abstract

This thesis will explore the deterministic dynamics of systems of coupled oscillators. In particular, the focus of the thesis will be concerned with the transport properties of these systems. Of interest is how particles work together, cooperatively, to achieve directed transport. For this reason, the strength of the coupling between the particles will serve as the main control parameter. Further, ensemble dynamics will serve to highlight some of the collective effects of these systems.

The thesis will be split into two parts. The first part will look at a class of autonomous Hamiltonian systems, while the second part will consider a class of driven and damped systems. A common feature of these systems is that they contain a spatially open component that will facilitate long range transport. More precisely, transport proceeds in a spatially symmetric and periodic multiple well potential. Thus transport will be characterised by particles overcoming successive energetic barriers created by the potential landscape.

The cooperative effects between the particles will become apparent in Part I when the autonomous Hamiltonian systems are considered. In the uncoupled limit the full systems decompose into two integrable subsystems and the dynamics are fully understood. However, the dynamics become more complicated when the particles are coupled. As these systems are conservative a coordinated energy exchange between the particles is often required for directed transport to ensue. Interestingly, these systems contrast well with the nonautonomous one and a half degree-of-freedom Hamiltonian systems, where transport occurs through intermittent periods of directed motion in
so-called ballistic channels. The autonomous two degree-of-freedom counterpart considered here relies on a rather different mechanism for directed transport that will be provided solely by regular structures in phase-space.

With the inclusion of external driving and damping (Part II) the transport dynamics are controlled by various coexisting attractors in phase-space. The nature and stability of these attractors is determined by the system parameters. As before, cooperative effects will play a key role when it comes to particle transport. Notably, it will be seen that coupling between the particles can result in a suppression of chaos that will allow for, for example, collective periodic motion of rotational type. Particular attention will be paid to the phase-space structures and how they change as the coupling parameter is varied.

Throughout the thesis these nonlinear systems, and their transport features, will be explored using analytical and numerical means. A number of model systems will also be introduced to further illuminate the systems dynamics.
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CHAPTER 1

Introduction

The topic of particle transport is often concerned with the movement of particles through potential landscapes. Studies of transport in systems often focus on how forces on the particles resolve themselves to allow for directed transport, i.e. net transport that is (on average) in one direction or another. Of particular interest is the ratchet effect: the possibility to obtain directed transport by using zero mean perturbations. The state of the art with respect to transport in spatially periodic systems out of thermal equilibrium was presented recently (Reimann, 2002).

Some of the earliest studies of particle transport were in the area of celestial mechanics, in an effort to understand, for example, the motion of planets orbiting a star. Since the advent of numerical computation (Zabusky, 1981), investigations into particle transport have increased at an almost exponential rate. This new tool has complemented analytical and experimental work already being carried out. In addition, the twentieth century saw the birth of new fields of research, fuelled by application areas such as Josephson junctions, cold atom systems, and Bose-Einstein condensates, where transport properties shed light on the features of these systems. Thus the study of transport properties is a very active area of research.
1.1 Hamiltonian Systems

Hamiltonian systems will form the backdrop for much of this thesis. It is therefore worthwhile to give a brief introduction to such systems now.

Hamiltonian systems are completely described by a single (scalar) function, usually given as \( H(p(t), q(t), t) \). This function is known as the Hamiltonian, where \( p(t), q(t) \in \mathbb{R}^N \) denote canonically conjugated momenta and positions, and \( t \) represents time. Here \( N \) represents the number of degrees-of-freedom. The notation \( p(t), q(t) \) serves to highlight that \( p, q \) are functions of time. For brevity the explicit time dependence will be omitted from now on. The state of the system is given as a point \( (p_1, p_2, ..., p_N, q_1, q_2, ..., q_N) \) in the \( 2N \)-dimensional phase-space.

From the Hamiltonian function, it is possible to derive the equations of motion (also known as Hamilton’s equation). They are defined by

\[
\begin{align*}
\dot{p}_i &= \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}(p, q, t) \\
\dot{q}_i &= \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}(p, q, t)
\end{align*}
\]  

(1.1)

(1.2)

where \( i \in [1, N] \). The Hamiltonian systems with no explicit time dependence are said to be autonomous. Such systems have the important property of conserving energy. That is, for \( H(p, q, t) = H(p, q) = E = \text{const.} \), the energy \( E \) remains invariant through the time evolution of the system. It is easy to verify this fact by taking the total derivative of the Hamiltonian:

\[
\frac{dH}{dt} = \frac{\partial H}{\partial t} + \sum_{i=1}^{N} \left( \frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{\partial p_i} \dot{p}_i \right).
\]

(1.3)

From Eq. 1.1 and Eq. 1.2, and given the fact that the Hamiltonian has no explicit time dependence, this reduces to
\[
\frac{dH}{dt} = \sum_{i=1}^{N} \left( \frac{\partial}{\partial q_i} \left( \frac{\partial H}{\partial p_i} \right) + \frac{\partial}{\partial p_i} \left( - \frac{\partial H}{\partial q_i} \right) \right) = 0. \tag{1.4}
\]

For autonomous systems the energy is an example of an integral of motion. Integrals of motion are functions of the \(2N\) phase-space variables

\[
F(p_1, ..., p_N, q_1, ..., q_N) = C = \text{const.,} \tag{1.5}
\]

such that \(F(\cdot)\) remains constant through the time evolution of the system. That is,

\[
\frac{dF}{dt} = 0. \tag{1.6}
\]

Integrals of motion, for autonomous and non-autonomous systems, have the important consequence of confining motion to lower dimensional surfaces in phase-space. Related to the idea of constants of motion is that of integrability. A system is said to be integrable if there exist \(N\) independent integrals of motion. In this case motion takes place on an \(N\)–dimensional surface in the \(2N\)–dimensional phase-space. Importantly, motion in an integrable system is either quasiperiodic or periodic. To see this requires passing, via a coordinate transformation, to a new set of variables known as action-angle variables (see Reichl (1992) for derivation of the action-angle variables). This change of variables, \((p, q) \rightarrow (J, \Phi)\), is important as the new Hamiltonian expressed in these variables depends only on the action variable \(J\), i.e. \(H(J, \Phi) = H(J)\). From this new set of variables one obtains \(N\) frequencies \(\omega_1, ..., \omega_N\) which define motion on a torus. If these frequencies are integer multiples of one another then the motion is periodic. However, if any of the frequencies are incommensurate, then the motion will be quasiperiodic. That is, if

\[
m\omega_i \neq n\omega_j \quad i \neq j, \tag{1.7}
\]
for some integers $m, n$ and $i, j \in [1, N]$ then motion on the torus is said to be quasiperiodic.

1.2 Transport in General

1.2.1 Individual Particles

A large portion of the literature has focused on the transport properties of individual particles. Mackay et al. (1984) carried out important work on transport in (autonomous) Hamiltonian systems (in this case, maps). In particular, they outlined the structures contained in a largely chaotic phase-space, most notably cantori and KAM-tori, that play a key role for the occurrence of transport. They showed that the particle flow through the partial barriers, created by cantori, was controlled by turnstiles that could trap particles in transporting channels. As an illustrative example, the phase-space of the standard map is shown in Fig. 1.1 (details of the standard map can be found in Reichl (1992), for example). Both chaotic and regular regions are clearly visible. In fact, magnification of any of the boundaries between regular and chaotic regions will reveal more intricate structures embedded in the chaotic regions. In particular, the hierarchy of cantori will be revealed through successive magnifications of particular regions.

Later, analogous features would take prominence in driven (non-autonomous) Hamiltonian systems (flows) (Yevtushenko et al., 2000; Denisov et al., 2002a). In many studies it has been shown that the emergence of a current is triggered by an external time-dependent field of zero mean. Important in this respect are the spatio-temporal symmetries (cf. § 1.5.1) of the system. With regard to the emergence of a non-zero current, all symmetries that, to each trajectory, generate a counterpart moving in the opposite direction need to be broken. Further, it has been shown that a mixed phase-space is required (Schanz et al., 2001). The mixed phase-space, con-
Figure 1.1: Illustration of a mixed phase-space where chaotic and regular regions coexist. The underlying map is the *standard map*.
taining regular and chaotic components allows for directed transport in the chaotic component of the phase-space. The regular and irregular components are separated by impenetrable KAM-tori which are in turn surrounded by a hierarchy of cantori. These cantori, although appearing to form closed curves, are interspersed by an infinite number of gaps, which allow particles to pass through and become stuck in *ballistic channels*¹ (similar to the turnstiles idea from maps). It is these sticking episodes that allow for directed transport (this is expanded upon in § 1.5.2). The general phenomena is sometimes called *intermittency* (Cvitanović et al., 2010).

The observation of a non-vanishing current, as an average velocity in coordinate-space, based on the chaotic ratchet effect as discussed in Flach et al. (2000); Denisov et al. (2002a,c,b) has even been extended to chaotic ratchet acceleration expressed in terms of an averaged velocity in momentum space (Gong & Brumer, 2004). In both cases the sum rule derived in Schanz et al. (2005) for the chaotic transport velocity in driven one-dimensional systems assures the existence of a persistent chaotic ratchet current.

The case of particles in non-Hamiltonian systems has also attracted considerable interest. While the Hamiltonian systems remain an active area of research, some have focused on less idealised systems that are dissipative (possibly including noise), and driven. Brownian motors extract work from thermal fluctuations in out-of-equilibrium conditions. With regard to transport under such thermal fluctuations, the ‘constructive role of Brownian motion’ is crucial (Astumian & Hänggi, 2002; Hänggi & Marchesoni, 2009). A particular type of Brownian motor is known as a Brownian ratchet. Motion in such ratchets is confined to a periodic and asymmetric potential (see Fig. 1.2 for an illustration of the ratchet potential), and in out-of-equilibrium conditions they

¹Ballistic channels exist inside the chaotic component of a mixed phase space at the boundary with the regular regions. Motion inside a ballistic channel is characterised by long periods of non-zero average velocity. In contrast, motion that takes place inside the chaotic component, but not at the boundary of a regular region, will usually have vanishingly small average velocity.
are able to rectify thermal fluctuations. Interestingly, under certain conditions, it is possible to derive analytical solutions pertaining to transport of Brownian particles via the *Gambler’s Ruin* model (Cheng et al., 2007). For Brownian ratchets, the broken spatial symmetry combined with external forces with time-correlations were shown to be sufficient ingredients for transport (Magnasco, 1993). The interdependence of the confining potential landscape and of the thermal fluctuations, for the emergence of transport, has further been studied (Malgaretti et al., 2012). Importantly, it was shown that the dual effect of the thermal noise and the ratcheting mechanism, which may by themselves be insufficient transporting mechanisms, can combine to produce conditions suitable for transport.

In general though, the dynamics of particle motion in periodic potentials at finite temperatures is an extensively studied field (Risken, 1989). In a similar domain, Hennig et al. (2009b) investigated the motions of driven, under-damped Brownian particles, evolving in a *washboard potential* (a spatially symmetric and periodic potential – see Fig. 1.2), under the influence of a time-delayed feedback term. They
found that, at finite temperatures, the time-delayed feedback term can in fact enhance the transport features of the system such that there is an increase in the overall net motion of the system, which is not observed when the feedback term is switched off. These results were related to a desymmetrisation of the relevant attractors supporting directed transport.

Transport of particles in potentials with multiple wells, at its most fundamental level, is characterised by escape processes. Thus it is important to understand the nature of particle escape over potential barriers. In determining escape phenomena, the most common approach is to look at the thermally activated escape processes of single particles out of metastable states. The cornerstone work by Kramers has instigated intensive research in this area (reviewed by Hänggi et al. (1990)). Briefly, thermally activated barrier crossings require a rare optimal thermal fluctuation that triggers an escape event. These works have been complemented by Hennig et al. (2008) who paid particular attention to the deterministic (noiseless) particle escape from a local confining potential well. The authors showed that for adiabatically slow modulations of the potential landscape all particles will escape from a potential well, in the same direction, and subsequently enter a regime of long lasting transients where the particles transport in a ballistic fashion, as described above.

Regarding mechanisms that allow for directed transport in a higher dimensional phase-space Reimann (Reimann, 2002) had this to say

> The situation in systems with a more than two dimensional phase-space (bringing along Arnold diffusion) has so far not been considered at all.

While this may no longer be strictly true, it emphasises that much work is still to be done in this area. Some of the work done in systems with at least two degrees-of-freedom are considered now.
1.2.2 Transport With Two or More Degrees-of-Freedom

Increasing the number of degrees-of-freedom to two (two and a half), and by consequence the dimension of the phase-space to four (five), by coupling two individual particles together adds further complexity to the system’s dynamics. For those studies which look at the transport features of systems of coupled oscillators, the objective is to investigate the conditions which lead to said transport features. In particular, for directed transport to occur, it is quite often the case that the two particles will work cooperatively to achieve this directed transport. Importantly, under the same conditions, a dimer (a compound made up of two particles) has distinct transport properties compared with those of the single particle (Heinsalu et al., 2008).

Dimer systems have been shown to exhibit a complicated dependence, with respect to observables of interest, on the coupling between the subsystems making up the dimer. For example, the value of the net transport for a dimer system can change erratically as the coupling parameter is varied (Hennig et al., 2009a). Similarly, Fugmann et al. (2008) considered the conservative and deterministic escape dynamics of two coupled particles out of a metastable potential. The scenario considered is such that neither particle can escape independently (on energetic grounds), and thus cooperation is required. It was shown that the escape times of the dimer out of the metastable state become severely inhibited for coupling strengths that are either too large or too small.

Further increasing the number of degrees-of-freedom makes analysis of these systems more problematic. Some of the already illusive phase-space structures become difficult, if not impossible, to detect. However, in spite of this, it is still possible to explore the transport properties in these higher dimensional systems. Taking a chain of linearly coupled units, each with its own local cubic potential, Hennig et al. (2007a,b) considered the conservative and deterministic escape of the chain from a metastable state. Interestingly, the initially injected energy is only sufficient for a fraction of the chain links to overcome the barrier height created by the cubic poten-
tial. However, working together the chain units reach a transition state that allows the whole chain to overcome the potential barrier and escape to infinity. Fugmann (2007) considered a similar problem for one- and two-dimensional chains. Beyond escape of a one-dimensional chain, Zheng et al. (2002) observed directed current for a chain consisting of one hundred units evolving in a spatially symmetric and periodic potential. The mechanism allowing for this unidirectional current is, they claim, the external driving that serves to break temporal symmetry of the system (see also § 1.5.1).

1.3 Anomalous Transport

For systems modelling the dynamics of particles evolving in periodic potentials, the inclusion of driving and damping can produce some interesting and unexpected behaviours. For such a particle, where the underlying potential is of the ratchet type and the driving is of zero average, Mateos (2000, 2001) observed a current reversal via an increase of the driving amplitude – that is, the current, going in one direction, passes through zero and changes direction as the driving amplitude is increased. A ratchet subjected to an unbiased external force that periodically modulates the inclination of the potential, is called a rocking ratchet. Current reversals in such a system are unexpected due to the inherent bias contained in the ratchet potential. In this situation, the current reversal, when it occurs, has been shown to coincide with a bifurcation from chaotic to regular motion (Mateos, 2000). In a similar study Mateos (2003) related current reversals to the basins of attraction for the system’s coexisting attractors that produce counterpropagating motion. This study differs from the previous two in that a current reversal is obtained through the appropriate selection of an initial condition, rather than through the modification of a control parameter. These studies have been extended to consider the case of two coupled driven and damped particles evolving in a ratchet potential (Vincent et al., 2010).
Not surprisingly, the addition of the second particle can have important consequences for the current reversals observed in the case of the single particle. It appears that current reversals exist for coupling strengths below some critical value. However, beyond this critical coupling strength, the particles become synchronous – the single particle dynamics are restored – and no further current reversals are observed. Little explanation is given as to why no further current reversals appear. However, from the Mateos (2000) study it is known that current reversals are restored, in the case of the single particle, for stronger driving amplitudes. In a separate study, Cubero et al. (2010) investigated the dynamics of a single particle evolving in a periodic and spatially symmetric potential landscape. In such a potential, there is no inherent bias with respect to transport. Thus, for a current to emerge at all, some symmetry of the system needs to be broken (such symmetries are discussed in detail in § 1.5.1). Cubero et al. (2010) achieved this by using a bi-harmonic driving term, resulting in a system that is driven out of equilibrium by an asymmetric external force. The authors provide evidence that current reversals, in this situation, are induced by the symmetry-breaking effect of the system’s damping.

Other types of counter-intuitive transport can be collected under the term negative mobility. To motivate this, let us consider two examples. The first, coined the Brazil nut effect, occurs when granular media of different sizes are mixed. Applying a rocking force to the mixture can cause the unexpected result that the larger granules rise (Mobius et al., 2001). Secondly, an effect known as induced demand can help explain, for example, the counter-intuitive rise in traffic when new roads are created (explanations include people wanting shorter journey times, access to better roads, etc). For particle transport, negative mobility also plays a role. In one article Eichhorn et al. (2005) gives an overview of this topic, together with a list of possible applications. In particular, they describe two types of motion of this kind; namely, absolute negative mobility (ANM) and differential negative mobility (DNM). For illustration, consider a simple system consisting of a single particle in equilibrium, which
has a spatially static homogeneous force $F$ applied. It is generally expected that the response of this system to the bias force $F$ is in the direction of, and proportional to, this force. However, for systems driven out of equilibrium (and possibly with the inclusion of noise), these new types of motion can be observed. ANM refers to motion whose response, on average, to the sufficiently small bias force $F$ is in the opposite direction of $F$. DNM on the other hand refers to motion that, although in the same direction as $F$, slows down as the magnitude of $F$ increases. These ideas have been expanded upon to further understand the response of these systems to noise (Speer et al., 2007a,b).

The case of coupled particles has also been considered. For under-damped particles evolving in spatially periodic and symmetric potentials, subjected to periodic driving and an additional static bias force, Mulhern & Hennig (2011) related the occurrence of negative mobility to a bifurcation from chaotic to regular motion. Further, a heuristic description of the mechanism that allows for such motion is outlined. In short, the particles must together work cooperatively in conjunction with the periodic driving so that ‘downhill’ motion is minimised, while ‘uphill’ motion is promoted. Thus, ‘uphill’ motion ensues. The corresponding solutions remain stable under low temperature fluctuations. In contrast, outside the observed windows of negative mobility, it is the chaotic dynamics that emerge resulting in motion that is in the same direction as the bias. A later investigation by Speer et al. (2012) can be considered as an extension of this study to the case of over-damped particles. Again, ANM was observed. They were able to prove that ANM is not possible for an over-damped dimer where the interaction potential is convex. That is, for a system of two coupled particles in the over-damped limit, subject to the forces discussed above, and with an interaction potential $W(x)$ such that

$$W''(x) > 0 \quad \forall x,$$

the possibility of ANM is excluded.
1.4 Transport in Irregular Domains

Extensions to studies of autonomous Hamiltonian systems of one-dimensional billiard chains have followed (Acevedo & Dittrich, 2003; Schanz & Otto, 2005). The necessity of creating chaos requires at least two degrees-of-freedom. As an example for such a system, a classical magnetic billiard for particles carrying an electric charge has been studied in Acevedo & Dittrich (2003). In order to break the time-reversal invariance, an external static magnetic field, penetrating the plane of motion perpendicularly, has been applied. In addition, achieving directed transport requires breaking of the remaining spatial symmetry which can be achieved, e.g. by properly placed asymmetric obstacles inside the billiard (Acevedo & Dittrich, 2003; Schanz & Otto, 2005). Uni-directional motion in a serpent billiard chain has been reported in Horvat & Prosen (2004).

Bunimovich (2001) introduced a novel class of billiard which he called the Mushroom Billiard. For an example see Fig. 1.3. Its novelty comes from the fact that it has the remarkable property of having a phase-space consisting of a single (regular) KAM-island and a single (chaotic) ergodic region. Such billiards offer insight into the dynamics of Hamiltonian system with a more complicated phase-space (see § 1.5.2). In fact Altmann et al. (2005, 2006) looked at the stickiness of chaotic trajectories to the single KAM island, using recurrence time statistics, in mushroom billiards. It was shown that the sticking episodes are facilitated by orbits known as marginally unstable periodic orbits. Marginally unstable refers to the fact that perturbations grow linearly (rather than exponentially) in time. These orbits, even though being of measure zero, govern the main dynamical properties of the system. Most notably, they are responsible for a power-law behaviour observed in the recurrence time statistics – something that is often related to the partial barriers created by cantori in a mixed phase-space.
1.5 Properties that Determine Transport Features

1.5.1 Symmetry Properties

A symmetry analysis of a system of equations can illuminate important transport properties. An important quantity related to transport is the time averaged, ensemble averaged, momentum. This is typically called the current. Let $p(t)$ represent the momentum of a particle at time $t$, then the current is given by

$$ J = \frac{1}{T} \int_0^{T} dt \left( \frac{1}{N} \sum_{n=1}^{N} p_n(t) \right) , $$

with $N$ being the number of initial conditions in the ensemble, and time $T$ taken in the asymptotic limit $T \to \infty$. There are other definitions of the current, that will be discussed later in the chapter, but this definition is useful in general. The direction and magnitude of the current is inextricably linked with a system’s symmetry properties.

To give an example, Flach et al. (2000) considered the symmetry properties of a
system consisting of a particle evolving in a spatially periodic potential subjected to driving and damping. The equation of motion is given by

\[ \ddot{X} + \gamma \dot{X} + f(X) + E(t) = 0. \tag{1.10} \]

Here \( E(t) = E(t + T) \) is a time-periodic external field of period \( T = 2\pi/\omega \) and frequency \( \omega \), and \( f(X) = f(X + 2\pi) \) is a periodic potential function. Both \( E(t) \) and \( f(X) \) are assumed to be bounded, and \( \max(|f(X)|) \sim 1 \). The authors defined two system symmetries related to the properties of the underlying potential and external field. These properties (shown in a modified form which allows for greater applicability – due to Lade (2010), for example) for a given function \( g(a) \) are

\[
\begin{align*}
g_s : & \quad g(a + \tau) = g(-a + \tau) \quad \text{for some } \tau \quad \text{(symmetric)} \\
g_a : & \quad g(a + \tau) = -g(-a + \tau) \quad \text{for some } \tau \quad \text{(anti-symmetric)} \\
g_{sh} : & \quad g(a) = -g(-a + \tau) \quad \text{for some } \tau \quad \text{(shift-symmetric)}
\end{align*}
\]

where \( g(a) \) can represent either a spatial or temporal function, i.e. the potential or the time-dependent external field, respectively. If \( f(X) \) is anti-symmetric, and \( E(X) \) shift-symmetric \((f_a\text{ and }E_{sh})\), then Eq. (1.10) is invariant under the symmetry \( \hat{S}_a : X \mapsto (-X + 2\chi), t \mapsto t + T/2 \) for some appropriate argument shift. In the dissipationless case, \( \gamma = 0 \), a second symmetry can be obtained. If \( E(t) \) possess the shift-symmetry \( E_{sh} \) then Eq. (1.10) is invariant under the symmetry \( \hat{S}_b : t \mapsto -t + 2\phi \), again for some appropriate argument shift.

It then follows that for a given trajectory \( X(t; t_o, X_0, P_0) \), \( P(t; t_0, X_0, P_0) \) with initial condition \( t_0, X_0, P_0 \), it is possible to generate new trajectories given by

\[
\begin{align*}
\hat{S}_a &: \quad -X(t + T/2; t_0, X_0, P_0) + 2\chi, -P(t + T/2; t_0, X_0, P_0) \quad \{\hat{f}_a, \hat{E}_{sh}\}, \\
\hat{S}_b &: \quad X(-t + 2\phi; t_0, X_0, P_0), -P(-t + 2\phi; t_0, X_0, P_0) \quad \{\hat{E}_s, \gamma = 0\}.
\end{align*}
\]

Importantly, these transformations change the sign of \( P \). This has the consequence
that the original trajectory, and the corresponding trajectory generated through the
symmetry transformation yield time-averaged values of $P$ that differ only by sign.
Going further, for a system with $S_a$ or $S_b$ symmetry, the net current will be zero as
each trajectory will have a counterpart that negates the others contribution to the
current. The implication being that in order to generate a non-zero current, both the
symmetries $S_a$ and $S_b$ need to be broken. Note that $S_a$ holds in both the dissipation
and the dissipationless cases, whereas $S_b$ holds only for $\gamma = 0$. Denisov et al. (2002a)
identified an additional symmetry, $\hat{S}_c$, of Eq. (1.10), this time in the over-damped
case where inertial effects become negligible, namely

$$
\hat{S}_c : X(-t; t_0, X_0, P_0) + \chi/2, -P(-t; t_0, X_0, P_0) \quad \{f_{sh}, E_a, m = 0\}.
$$

It is worth noting that the symmetries $\hat{S}_a, \hat{S}_b$ and $\hat{S}_c$ require that the time-dependent
external field satisfies certain properties. Thus, an appropriate choice of $E(t)$ can be
sufficient to break all three symmetries.

Yevtushenko et al. (2000) investigated the symmetry properties of the Hamiltonian
version of Eq. (1.10) ($\gamma = 0$), where the underlying potential is spatially periodic and
symmetric. A lowering of the dynamical symmetry, controlled by the phase of the
external field, leads to a directed current.

### 1.5.2 Ballistic Transport

Others have focused on the dynamical mechanisms that allow for a directed current
in a mixed phase-space. While the appearance of a dc-output can be expected using
symmetry analysis, its appearance and magnitude are due to dynamical mechanisms
of motion inside the stochastic layer. Denisov & Flach (2001) looked at the structures
in phase-space and considered how they influence the magnitude and direction of
current. To ensure that the appropriate symmetries were broken, thus allowing for a
directed current, they chose the external field
\[ E(t) = E_1 \cos(t) + E_2 \cos(2t + \phi), \] (1.11)

where \( E_2 \neq 0 \) and \( \phi \neq 0, \pi \). The phase-space of this system is characterised by a stochastic layer which emanates from the separatrix of the unperturbed system \((E_1 = E_2 = 0)\). Inside the stochastic layer there exists a hierarchical structure of resonance islands that are responsible for the creation of ballistic channels in phase-space. That is, the resonance islands form partial barriers such that when a particle enters a ballistic channel it may be stuck there for large durations, thus contributing to an overall non-zero net current (see Fig. 1.1). The authors relate the emergence of a directed current to a desymmetrisation of the ballistic channels bringing the particles in opposite directions. Going further, they analytically derive an expression for the current from the geometry of the phase-space. In particular, each resonance island has associated to it a winding number \( \omega_i \), a probability of ‘sticking’ to the resonance island \( \rho_i \), and mean sticking time \( \langle t_i \rangle \). In addition the mean time between sticking episodes is \( \langle t_r \rangle \). Finally, they define the current as

\[ J = \frac{\sum_{i=1}^{N} \omega_i \rho_i \langle t_i \rangle}{\sum_{i=1}^{N} \rho_i \langle t_i \rangle + \langle t_r \rangle} \] (1.12)

where \( N \) is the number of resonance islands. This definition of the current suffers two limitations. Firstly, the four unknowns in the equation will, in general, need to be computed numerically. The second is that there may be resonances of all orders. To even locate resonances of increasing order becomes computationally impractical. However, this does not pose much of a problem as it is only a few resonance islands that are relevant for obtaining the net current. Higher order resonances have sticking times that are close to zero and therefore their contribution to the net current is negligible.
1.5.3 Chaotic Motion

All of the studies discussed above look at systems with at least (effectively) three variables. Thus the dynamics of these systems can be chaotic. Although chaotic motion seems to be inherently counter-productive with respect to net motion in one or another direction, it can, for example, allow trajectories to visit (transporting) ballistic channels associated to resonance islands with non-zero winding numbers (Schanz et al., 2005). However, such ballistic channels will only exist in non-hyperbolic systems: systems that contain mixed regular and chaotic regions (cf. § 1.5.2). These chaotic regions are born out of (nonintegrable) perturbations to an integrable system, with the strength of perturbations determining the prevalence of chaos. This is true in general, i.e. (nonintegrable) perturbations to an underlying integrable system are the source of chaos.

One method for proving that a bifurcation from regular to chaotic motion occurs is through the homoclinic Melnikov method. This perturbational approach determines the first transversal intersection of the stable and unstable manifolds, related to some hyperbolic fixed point (or periodic orbit), that separate due to perturbations. For planar systems this method has been described in many texts (for example, Sanders et al. (2007)). Later, the Melnikov method was modified so as to be applicable to higher dimensional systems (Wiggins, 1990).

The particular case of coupled oscillators has also been subjected to a homoclinic Melnikov analysis. Yagasaki (1999b), using as an example two coupled Duffing oscillators, gave a thorough description of the unperturbed geometrical structure of phase-space. The author then proceeded to derive, for the perturbed system, homoclinic bifurcation results for orbits homoclinic to periodic orbits using a modified form of Melnikov’s method.

Out of the perturbational regime a particular tool is quite often used to quantify chaos in a system. This tool is the Lyapunov exponent and there is one such exponent
for each direction in phase-space (Guckenheimer & Holmes, 1983). The basic idea of the Lyapunov exponents is to measure the rate of separation of neighbouring trajectories in a phase-space direction. Formally, let \( e_1(t), e_2(t), \ldots, e_m(t) \) be the eigenvalues of the variational equation \( \Phi_t(x_0, t_0) \) of a flow, where \( x_0, t_0 \) are the initial condition and time respectively, and \( m \) is the dimension of phase-space. Then the Lyapunov exponents are defined as

\[
\lambda_i = \lim_{t \to \infty} \frac{1}{t} \log(|e_i(t)|), \quad i = 1, 2, \ldots, m.
\] (1.13)

A positive Lyapunov exponent indicates that neighbouring trajectories diverge at an exponential rate in a phase-space direction (a hallmark of chaos), whereas a negative exponent indicates stability in that phase-space direction. There is also a zero exponent which indicates a steady state where there is no contraction or expansion.

In many cases it is sufficient to calculate the maximal Lyapunov exponent (Sandri, 1996) as this is often enough to determine whether or not a system is chaotic. It is calculated as follows. Starting with two ‘close’ neighbouring trajectories separated at time \( t_0 \) by a small distance \( d_0 \) in phase-space, the maximal Lyapunov exponent is given by

\[
\lambda = \lim_{t \to +\infty} \frac{1}{t - t_0} \ln \frac{d(t)}{d_0}
\] (1.14)

where \( d(t) \) is the phase-space distance between the two orbits at time \( t \).

In general though, more information can be obtained by determining the full Lyapunov spectrum (the individual exponent for each phase-space direction). Numerically, this is more challenging than computing the single maximal Lyapunov exponent. The method is well described by Wolf et al. (1985). It requires (for flows) integrating a system’s equations of motion ignoring some predefined transient period. Simultaneously, the system’s linearised equations of motion are integrated for \( n \) different initial conditions defining \( n \) orthogonal vectors that form a basis for the
vectors in phase-space. Then, all of the exponents are calculated for the duration of simulation with appropriate averaging carried out. One of the key difficulties with this method is that, over time, all of the vectors tend to align along the direction of the maximal Lyapunov exponent. To circumvent this problem repeated use of some orthonormalisation tool, such as Gram-Schmidt Orthonormalisation (Chow, 2000), is required. This will keep the vectors properly aligned and will avoid divergence in the magnitudes of the vectors.

By determining the full spectrum of Lyapunov exponents one is able to characterise a new type of motion – hyperchaos. This term was first introduced by Rössler (1979) to describe a highly unstable form of chaotic motion. It occurs when at least two of a system’s Lyapunov exponents become positive indicating exponential growth in more than one direction in phase-space. That is, neighbouring trajectories will separate at an exponential rate along at least two phase-space directions.

The transition from chaos (one positive Lyapunov exponent) to hyperchaos (more than one positive Lyapunov exponent) has attracted interest in recent years. Using as an illustrative example a system consisting of two coupled logistic maps, Kapitaniak et al. (2000) provided evidence that this transition occurs as the result of changes in the stability of an infinite number of unstable periodic orbits embedded in the chaotic attractor. That is, in the neighbourhood of the chaos–hyperchaos transition infinitely many unstable periodic orbits (one positive Lyapunov exponent) change their stability type to become repellors (two positive Lyapunov exponents). Extending this work to the case of flows, Yanchuk & Kapitaniak (2001) examined the transition in two coupled Rössler systems. As was observed for maps, the transition was related to a change in stability of the infinite number of unstable periodic orbits embedded in the chaotic attractor.
1.6 Chapter Summary

Particle transport has been an active area of research over the years. This chapter has outlined some of the important works related to particle transport. To understand transport effects in systems modelling particle movement through potential landscapes requires a thorough analysis of the underlying system. Most notably, the symmetry properties can be extremely insightful. In addition, interesting transport effects can occur. It may be that directed transport can be observed at all – *Brownian ratchets* – or, something rather different such as *absolute negative mobility* where, counter-intuitively, transport proceeds in a direction opposite to some applied bias force. However, it is clear that these systems provide a rich source of complex and interesting dynamics that warrant further study.
Preface

The focus of this thesis is on the deterministic transport properties of systems of two coupled oscillators (particles). In particular, much attention will be given to the relationship between various transport scenarios and the coupling between the particles. Notably, the nature of the interaction between the particles that allows for directed transport (on average) will be scrutinised.

Much of the literature to-date has focused on the transport properties of nonautonomous single particle systems where transport proceeds in the mixed phase-space due to intermittent periods of regular motion caused by sticking episodes of particles to islands with non-zero winding number. Others have looked at, for example, the escape dynamics of larger chains of coupled unit out of metastable potentials. However, in such systems it becomes increasingly difficult to produce analytical and numerical results related to particle transport and current. Although, this is not impossible.

The work presented here serves as a bridge between single particle systems and many particle systems. Importantly, two particle systems are the first non-trivial step from the lower of these limits, bringing with it new types of motion, such as hyperchaos, that have important implications when it comes to transport. More than that, the work presented in this thesis will explore novel mechanisms pertaining to directed transport that are a direct consequence of the interaction between the
particles.

The thesis is split into two parts. The first – Chapters 2–4 – will explore autonomous Hamiltonian systems, while the second – Chapters 5–6 – will consider nonautonomous driven and damped systems. Throughout, both analytical and numerical results will be used to gain a fundamental understanding of these systems and their related transport properties.

In Chapter 2 some of the techniques that will be used at various stages of the thesis will be presented by way of example. These include Poincaré surface of section, and calculation of the current. The example will be a spatially symmetric system containing two open components allowing that either particle can undergo directed transport. By way of symmetry analysis, it is clear that if a constant energy surface is entirely populated by initial conditions then no current can emerge. However, this may not be the case for other, more physically relevant, sets of initial conditions. For one such set, some qualitatively different transport scenarios are outlined and their relation to the net current described. As a general point for the class of systems discussed in Part I, the mechanism promoting directed transport in these systems is quite different from systems where transport proceeds over finite periods in so-called ballistic channels, each period being separated by an interval of chaotic motion. The novel mechanism for transport presented here, where chaos is required only in a transient period of the dynamics (after which transport is provided solely by regular structures), will be illustrated and the implications discussed.

Chapter 3 is dedicated to a thorough symmetry (spatial and temporal) analysis of the general underlying class of Hamiltonian. While systems, for a given parameter set, may exhibit directed transport for specific initial conditions, with respect to ensembles the net flow might be zero. This chapter will explore how sets of localised initial conditions affect the overall net flow. In short, it will be shown that these sets of initial conditions can be enough to allow for the generation of a non-zero current, as long as a spatial symmetry of the system is in some way violated.
The inclusion of an interaction potential alters the location of a system’s equilibria. In Chapter 4 the location and properties of these equilibria will mapped out and discussed, using as examples the model systems presented in the previous chapters. Of interest is how these equilibria change as the strength of the interaction between the subsystems increases. Furthermore, when the two particles are decoupled, splitting the system into two integrable subsystems, the stable and unstable manifolds emanating from the hyperbolic fixed points coincide in phase-space, and thus the motion is regular. However, for non-zero interactions these manifolds separate. For strong enough coupling they can subsequently intersect non-transversely allowing for chaotic motion and the emergence of phenomena such as current reversal and suppression. This will also be discussed in detail.

Turning to Part II, the driven and damped dynamics of two interacting particles evolving in a symmetric and spatially periodic potential is considered. The latter is exerted to a time-periodic modulation of its inclination. In Chapter 5 this system is subjected to a perturbational analysis. Using Melnikov’s homoclinic method, the parameter regime for which the presence of transverse homoclinic orbits and homoclinic bifurcations for weak coupling is guaranteed, is determined. In addition, for directed particle transport mediated by rotating periodic motion, exact results regarding the collective character of the running solutions are derived.

Moving away from the perturbational regime, in Chapter 6 a thorough numerical study is used to further highlight the effects induced by the interaction between the particles. Two key points emerge. Firstly, working cooperatively the particles are able to suppress the effects of chaos. Secondly, the regime of hyperchaos – determined by calculating the full Lyapunov spectrum – coincides with the regime of zero current. Strikingly, even in the presence of chaos (characterised by one positive Lyapunov exponent) a non-zero current can still be observed.

The thesis is organised as follows: In Part I the autonomous Hamiltonian systems are considered. This part begins with an introduction where the class of system under
investigation is defined explicitly, and some of its general properties are discussed. Chapters 2–4 then follow where the content is as described above. In Part II the driven and damped systems are considered. Similarly, the class of system will be defined and its general properties outlined. Chapters 5–6 then follow with content as described above. To conclude the thesis, there will be a summary describing some of the main results. In addition, some areas requiring further work are outlined.

Almost all of the results presented here have been published. In particular, Chapters 2-4 are based on results contained in Hennig et al. (2010a,b); Mulhern et al. (2011); Burbanks et al. (2012), and Chapters 5-6 are based on results found in Hennig et al. (2011b); Mulhern et al. (2012)†.

Technical Considerations

With regard to the calculation and presentation of numerical results, the software used was all open-source software, such as Python, GNU Compiler Collection (GCC), Gnuplot and Paraview. Where numerical results are shown they were obtained from programs that were written by the author specifically for the problems considered in this thesis. Two main programming languages (including relevant libraries) were used for the various numerical tasks carried out in this thesis. These were C++, the primary language used, and Python. Secondly, for the graphical illustration of the numerical results all plots were produced with (primarily) Gnuplot, and Paraview. The actual thesis was prepared using the \LaTeX\ typesetting tool.

†Mulhern et al. (2012) has been submitted for publication.
Part I

Transport in Autonomous Systems
Introduction

In this part we will explore autonomous Hamiltonian systems modelling two coupled particles. The guiding aim is to understand the conditions under which directed transport in phase-space is supported. In particular, analytical and numerical results will be produced illustrating the effects that the interaction between the two particles has on the direction and velocity of transport.

The Hamiltonian systems discussed here will be of the form:

\[ H(p, q) = \frac{p^2}{2} + \frac{P^2}{2} + U(q) + V(Q) + H_{\text{int}}(q, Q), \]  

(I.1)

where \( p = (p, P) \in \mathbb{R}^2 \), \( q = (q, Q) \in \mathbb{R}^2 \) are the canonically conjugated positions and momenta of coupled particles. Further, we will assume from now on that these particles are of unit mass. The particles evolve in a potential given by \( U_{\text{eff}}(q) = U(q) + V(Q) + H_{\text{int}}(q, Q) \), where \( U(q) \) and \( V(Q) \) are positive semi-definite functions, and in addition, are coupled via an interaction potential \( H_{\text{int}}(q, Q) \). It may be the case that \( U \) and \( V \) describe the same potential landscape. However, to keep the results as general as possible, we consider both cases, i.e. when the potential landscapes are the same, and also when they differ. Crucially, a prerequisite for the occurrence of transport is that these systems contain an open component. That is, on surfaces of constant energy the system must be unbounded in at least one of the spatial coordinates, thus allowing for the possibility of unbounded and directed transport. Therefore, we assume that all systems explored here contain an open component. The equations of motion, corresponding to this class of Hamiltonian systems, are given by

\[ \ddot{q} = -\frac{\partial U_{\text{eff}}(q)}{\partial q} \quad \& \quad \ddot{Q} = -\frac{\partial U_{\text{eff}}(q)}{\partial Q}. \]  

(I.2)

Throughout the coming chapters we will use example systems to develop and illustrate theory that can be applied to the general class of systems described above.
While some methods have been used to obtain results that are system specific, these methods are applicable in general to the class of systems given above (cf. Eq. (I.1)).

Before moving onto the first chapter, it is worthwhile discussing a particular potential landscape that will be used in all of the coming chapters (including those in Part II of this thesis). This potential, often called the \textit{washboard} potential, is periodic (of period 1) and spatially symmetric (see Fig. 1.2 for an illustration). It is described by the equation

\[
U(q) = U(q + 1) = \frac{1 - \cos(2\pi q)}{2\pi}.
\]  

(I.3)

\(U(q)\) has minima at \(q_{\text{min}} = n\), with \(U(q_{\text{min}}) = 0\), and maxima at \(q_{\text{max}} = n + 0.5\), with \(U(q_{\text{max}}) = 1/\pi\, (\approx 0.318)\), where \(n \in \mathbb{Z}\). As mentioned, the potential is spatially symmetric, i.e. \(U(q) = U(-q)\).

For now let us suppose that a single particle is evolving in a washboard potential with no external forces present. The occurrence of transport can then be viewed as a string of consecutive escape processes where the particle overcomes the potential barriers located at \(q_{\text{max}}^{n+0.5}\) \((n \in \mathbb{Z})\) with increasing \(|n|\). The only requirement for directed transport is that the system possesses a sufficient amount of energy so that the particle can overcome these barriers.

An analogous statement regarding transport can be made for the case of two coupled particles. However, directed transport in this case may require not just a sufficient amount of system energy, but also a coherent energy exchange between the particles. This will be elaborated upon in the next section. To conclude this section an interaction potential used in the coming chapters is presented and its properties briefly discussed. The interaction potential is of the form

\[
H_{\text{int}}(q, Q) = D \left[1 - \frac{1}{\cosh(q - Q)} \right],
\]  

(I.4)
which is dependent on the distance $d = |q - Q|$. The strength of this coupling is regulated by the parameter $D$. Like the washboard potential, the interaction potential is also spatially symmetric — $H_{\text{int}}(q, Q) = H_{\text{int}}(-q, -Q)$. It is important to note that the gradient $\frac{dH_{\text{int}}(x)}{dx}$ goes to zero asymptotically, i.e. as the relative distance $|q - Q|$ increases, the related interaction forces, $\partial H_{\text{int}}/\partial q$ and $\partial H_{\text{int}}/\partial Q$, vanish asymptotically, allowing for transient chaos (Bleher et al., 1990; Contopoulos et al., 1993; Zaslavsky, 1985, 1998). That is, for large distance $|q - Q| \gg 1$, the interaction vanishes with the result that the two degrees-of-freedom decouple, rendering the dynamics regular. This is crucial for what will be presented in the coming chapters.

Part I is organised as follows. Throughout the thesis a number of model systems will be used to highlight/extract certain features of the class of system described by Eq. (I.1). The first of these models will be introduced in Chapter 2. Using a number of classical techniques, and some bespoke, this model will be thoroughly examined. Chapter 3 takes an indepth look at the symmetry properties of Eq. (I.1). In particular, this chapter will look at a mechanism that breaks the spatio-temporal symmetries of the system. This analysis will be aided by a second model system, which will also be introduced. Finally, using the two previously introduced models, Chapter 4 will then look at the system’s saddles, and their manifolds, and explore how they are affected by the coupling between the two subsystems.
CHAPTER 2

General Methods

Transport in autonomous Hamiltonian systems is remarkable due to the fact that a system requires no additional input of energy, in the form of an external (time dependent) drive for example, for said effect to occur. Rather an internal energy distribution must take place before particle transport can take place. This effect is even more remarkable in systems of coupled particles when the system’s energy does not suffice to allow that both particles can undergo rotational motion* at the same time. In this case the subsystems, related to each particle, must work cooperatively to achieve transport. In this chapter it will be shown that the strength of the coupling between the subsystems is crucial to the resulting dynamics. More than that, some general features of systems of coupled oscillators will be exposed.

This chapter also introduces numerous techniques that will be used throughout this thesis. These techniques will be illustrated using a model system that contains one of the key components for transport. That is, it contains an open component in at least one of the coordinates. In fact, for this model both spatial components are open allowing the possibility that either (or both) particles can undergo directed transport. This is not always the case, as will be seen in Chapter 3.

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*In this thesis rotational motion will refer to motion where a particle(s) overcomes consecutive potential barriers in a periodic fashion.
2.1 Spatially Symmetric Model (Model One)

Let us now introduce the model that will be used throughout this chapter. This model is minimal in two respects. The first is that $U$ and $V$ describe the same potential landscape – the so-called washboard potential. The second is that this system contains only one parameter, namely the parameter that regulates the strength of the bond between the two particles. Thus, there are two particles evolving in the washboard potential (Eq. (I.3)) that are coupled via the interaction potential (Eq. (I.4)). An example of the effective potential for the system described by the equation

$$U_{\text{eff}}(q) = U(q) + U(Q) + H_{\text{int}}(q,Q),$$

for coupling parameter $D = 0.58169$, is shown in Fig. 2.1 with $-2.5 \leq q \leq 2.5$ and $-2.5 \leq Q \leq 2.5$.

We see energies in the potential ranging from 1.21 (dark orange) to 0 (dark blue). Crucially, along the diagonal (blue area) exists the interaction region which is where the complexity in the system is manifested. Moving away from this diagonal, the interaction between the particles becomes weaker with growing distance $|q - Q|$.

The equations of motion are given by

$$\ddot{q} = -\sin(2\pi q) - D \left[ \frac{\tanh(q - Q)}{\cosh(q - Q)} \right],$$

$$\ddot{Q} = -\sin(2\pi Q) + D \left[ \frac{\tanh(q - Q)}{\cosh(q - Q)} \right].$$

For the numerics in the coming sections the initial set-up is as follows. The two particles will be separated by a sufficient distance such that they are effectively uncoupled, i.e. the energy contained in the interaction potential saturates: $E_{\text{int}} \approx D$. 
2.1. SYMMETRIC MODEL

Figure 2.1: Top: Plot of the effective potential \((D = 0.58169)\). The colouring indicates the potential energy: blue being regions of low energy, and red those of higher energy. The blue region is the so-called interaction region where the energy exchange between the particles is most pronounced. Bottom: This figure, showing a profile of the above figure, highlights the changes to the effective potential induced by the interaction potential.

One particle will be situated at the origin, while the other particle will be in a potential well that is sufficiently far from the origin, so that the effect of one particle on the other is almost negligible. Further, the particle at the origin will be at rest. The additional particle will be given an initial velocity that sees it move towards the particle at rest (these particles will henceforth be called particle \(A\), associated with
2.1. SYMMETRIC MODEL

the variables \((p, q)\), and particle \(B\), associated with the variables \((P, Q)\), respectively). Of course, the energy supplied to particle \(A\) must be greater than that required to overcome potential barriers of the washboard potential – that is \(E_A(0) > E_b = 1/\pi\), where \(E_A(0)\) is the energy possessed by particle \(A\) at time \(t = 0\) and \(E_b\) is the barrier height of the washboard potential. Thus, as the relative distance \(|q - Q|\) decreases, the energy exchange becomes more pronounced (depending on the value \(D\)) and the system dynamics become more complex.

For \(D \neq 0\) the particles can interact via the interaction potential and exchange energy. This exchange will excite the additional (initially resting) particle and, to varying degrees, influences the motion of the particle that has entered the interaction region. Again, it is important to note that both components of this system are open and thus it is feasible that either particle will escape. For large \(|q - Q| \gg 1\) the interaction between the particles vanishes, and again the dynamics is represented by regular rotational motion (assuming sufficient system energy). For the systems considered here, the energy will be kept sufficiently low such that the possibility of both particles escaping independently is excluded (for more see § 4.2), and the cooperative effects between the particles come to the fore.

As mentioned earlier, the initial conditions for particle \(B\) will be \(Q = P = 0\). The particle \(A\) starts as a virtually free particle in the asymptotic region, i.e. it approaches the interaction region from a far distance. The initial amount of energy \(E = 0.9\) lies above the highest possible energy of the saddle-centre points but, for not too low coupling, below almost all of the saddle-saddle points of the effective potential (see further in § 4.2). The initial positions of the particles \(A\) are contained within the well whose minimum is located at \(q \simeq -25\) and the corresponding initial momenta are determined as those points populating, densely and uniformly, the level curve

\[
E = \frac{1}{2}p^2 + U(q) + H_{\text{int}}(q, 0),
\]  

(2.4)
in the $(q,p)$-plane. Asymptotically, the interaction potential attains a value approaching $D$. Therefore, as the particles begin in the asymptotic region and as the initial conditions depend explicitly on $D$, no two sets of initial conditions will be the same. Two examples of these initial conditions are shown in Fig. 2.2. The energy will be fixed at $E = 0.9$, which is less than three times the barrier height of the washboard potential, $E_b = 1/\pi \approx 0.3183$. It should be emphasised that for particle $B$ to escape, it must gain a sufficient amount of energy from its interaction with particle $A$. With no interaction this system will contain a strong positive current, as particle $A$ can escape to infinity feeling no effect from particle $B$. It is worth adding that for these initial conditions with $D \neq 0$ the problem becomes a particle scattering problem with the stationary particle playing the role of the scatter.

There are a number of questions that will be addressed: Firstly, can particle $B$ gain enough energy to escape from its starting potential well, or is particle $B$’s presence of little or no consequence to the overall dynamics of the system? Secondly, in the case that particle $B$ does escape, what subsequently happens to both particles? Finally, assuming that particle $B$’s presence is significant, can it influence the dynamics in such a way that there is a reversal of the direction of the current, or even a suppression.
2.1. SYMMETRIC MODEL

of the current? These questions will be answered in the subsequent sections.

To partially answer the first and second questions, some of the qualitatively different transport scenarios that are present in this system by varying the strength of the coupling parameter $D$ will be illustrated. Before this however, it is useful to present a table of $D$ values that will be frequently used in this chapter along with their respective currents. Particle current is assessed quantitatively by the mean momentum, which is defined by taking the averaged momentum of an ensemble of particles, i.e.

$$\bar{p} = \frac{1}{T_s} \int_0^{T_s} dt \langle p(t) \rangle,$$  \hspace{1cm} (2.5)

where $T_s$ is the simulation time, and the ensemble average is given by

$$\langle p(t) \rangle = \frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{2} p_{i,n}(t),$$  \hspace{1cm} (2.6)

with $N$ being the number of initial conditions. The current, along with details of the calculation, will be discussed in detail in § 2.2. Below is a table of representative coupling strengths with their respective current values.

<table>
<thead>
<tr>
<th>$D$</th>
<th>$\bar{p}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.925</td>
</tr>
<tr>
<td>0.5613</td>
<td>-0.239</td>
</tr>
<tr>
<td>0.5617</td>
<td>0.262</td>
</tr>
<tr>
<td>0.5672</td>
<td>0.009</td>
</tr>
<tr>
<td>0.58169</td>
<td>-0.0001</td>
</tr>
</tbody>
</table>

Fig. 2.3 contains plots showing the temporal evolution of the coordinates $q, Q$ for the five $D$ values contained in the table. For comparison, for each $D$ value, the initial positions of the pair of particles will be the same, i.e. with $q(0) = -25.5$ and $Q(0) = 0$, and the initial momentum $p(0)$ of particle $A$ follows from the relation given
in Eq. (2.4), while particle $B$ has zero momentum, $P(0) = 0$. Slightly altering these initial conditions can have a large impact on the path that the particles will take, as for a large range of the coupling strength the dynamics is chaotic. In addition, for the same $D$ values, Fig. 2.4 illustrates the time evolution of the partial energies which are defined as

$$E_1 = \frac{1}{2} p^2 + U(q) + \frac{1}{2} H_{\text{int}}(q, Q),$$

(2.7)

$$E_2 = \frac{1}{2} P^2 + U(Q) + \frac{1}{2} H_{\text{int}}(q, Q),$$

(2.8)

with $E_1$ and $E_2$ being the partial energies of particles $A$ and $B$ respectively, and with the interaction energy being divided evenly between the particles. From conservation of energy, the quantity $E = E_1 + E_2$ remains constant. It is important to note that as $D$ increases so does the initial amount of energy held in the interaction potential therefore giving less portion of the total energy to the first two terms of the energy of particle $A$ in Eq. (2.7). In fact, there exists a critical coupling strength $D_c$ such that, for $D > D_c$ and with the initial conditions described above, neither particle can escape from its starting potential well. A more rigorous explanation of this is contained in Theorem 2.1 and the subsequent discussion.

The $D$ values in the table above have been chosen as they represent, in addition to typical system dynamics, transport scenarios with varying contributions to the net current. With $D = 0.3$ (Figs. 2.3a, 2.4a) we see that particle $A$ is able to pass straight through the interaction region almost unscathed. Particle $B$ does receive some energy from the interaction, but this energy only allows for small oscillations about its starting position. This set-up favours a strong, positive current. With regard to particle $B$ leaving its initial potential well, there appears a blow-up at $D \approx 0.562$, after which we can expect both particles to travel multiple potential
wells together. As can be seen in Fig. 2.3b, 2.3c, both with $D < 0.562$, particle $B$ can largely influence the path of particle $A$ without actually leaving its starting potential well. Setting $D$ to 0.5613 (Fig. 2.3b, 2.4b) we see that the dynamics of the system is quite different. The interaction between the particles is such that particle $A$ can pass through the interaction region (to a certain extent) and subsequently be pulled back, escaping in the negative $q$ direction and thus contributing to current reversal. Again particle $B$ receives little energy from the interaction as can be seen in Fig. 2.4b. A similar phenomenon can be seen for $D = 0.5617$ (Fig. 2.3c, 2.4c). This time particle $A$ oscillates around $q = 0$ a number of times before escaping in the positive $q$ direction maintaining the original direction of the current. Some of the most interesting behaviour observed in this system can be seen in the remaining two figures. Figs. 2.3d, 2.4d show a trajectory with $D = 0.5672$. There are number of striking things that can be noted about this trajectory. Firstly, the duration of time that the trajectories ‘stick’ together before one escapes. In this case particle $B$ escapes in the positive $q$ direction. This is substantially longer than the escape times presented in the previous figures. Also, both particles take excursions to the left and right before the escape of particle $B$. However, the most notable thing about this figure is that it is particle $B$ that escapes, not particle $A$ as for the previous $D$ values. Thus, particle $B$ is able to gain enough energy to escape from its starting potential well, and subsequently from any force that it feels from particle $A$. Particle $A$ has sacrificed its energy and has become trapped. This situation describes an interchange of the roles played by particles, with the initially free particle becoming trapped and the initially trapped particle becoming free. The final figures (Fig. 2.3e, 2.4e), with $D = 0.56169$, show similar behaviour in that the particles seem to ‘stick’ together. However, neither particle escapes, but instead are, in some sense, stuck to each other for the duration of the simulation. This is a process known as dimerisation, where the particles, each initially acting as a monomer, form a bound unit. This process is evident in some of the previous figures, however in this case, the process is permanent. Both particles undergo large excursions, closely following the line $q = Q$. It can be
seen in Fig. 2.4e that, for this particular $D$ value, the particles are in a continual and most importantly, a substantial energy exchange. This allows the particles to travel together in an erratic fashion undergoing multiple changes of direction and visiting multiple potential wells. Although an independent escape for one of the particles remains a statistical possibility, it requires an optimal energy fluctuation that sees one particle sacrifice all of its energy to the other. This is highly unlikely given the fairly strong coupling between the particles.

A characteristic of each figure is that when particle $A$ enters the interaction region there is a slight increase in its momentum. This acceleration is due to the dip in the potential landscape, created by the interaction potential. Particle $A$ thus usurps some of the energy contained in the interaction potential. Importantly, the escape of one particle at the expense of the other, and therefore an increase in the distance between the particles, restores the initial amount of energy contained in the interaction potential.

### 2.2 Particle Current

We now consider the current induced by directed particle transport. For the calculation there were $N = 10^3$ initial conditions. To reiterate, the initial conditions are the following: There is an initially stationary particle ($P = Q = 0$), and a transporting particle with initial momentum and position obtained from Eq. (2.4) where $q \in [-25.5 : -24.5]$. The system energy is $E = 0.9$. Each initial condition was observed for a simulation time $T_s = 10^5$. The simulation time exceeds by far the time required for a single particle to escape from a well of the washboard potential. Further, $T_s = 10^5$ is equivalent to almost $4 \times 10^4$ times the period of harmonic oscillation, $T_b$, near the bottom of the washboard potential. That is, $T_s \gg T_b = \frac{2\pi}{\omega_b} = \frac{2\pi}{\sqrt{2\pi}} = \sqrt{2\pi}$, where $\omega_b$ is the frequency of harmonic oscillation near the bottom of a well of the
Figure 2.3: Example trajectories using a range of different $D$ values. The red line shows the temporal evolution of Particle $A$, while the blue line shows the time evolution of particle $B$. The initial conditions for each trajectory are chosen as $q(0) = -25.5$, $Q(0) = P(0) = 0$. $p(0)$ is obtained from Eq. (2.4). Note the different time-scales.
Figure 2.4: Partial Energies of particles $A$ and $B$, defined by Eq. (2.7) and Eq. (2.8) respectively, corresponding to the trajectories in Fig. 2.3. Again, the temporal evolution of particle $A$ is shown by the red line, and particle $B$ by the blue line. Note the different time-scales.
With regard to the actual numerical simulations (Part I & Part II), these were carried out using a fourth order Runge-Kutta method (Press et al., 1992) with a step size $dt = 0.01$. A transient period of $t_{\text{trans}} = 5 \times 10^4$ was ignored in the hope that the trajectories have approached their final state. Further, as these are autonomous Hamiltonian systems (Part I only), conservation of energy is guaranteed. To ensure this, conservation of energy was monitored for the entire simulation, to a high degree of accuracy, at each time step.

Fig. 2.5 shows the current, as defined in Eq. (2.5), for the system as a function of $D$. Strikingly one notices that there are intervals for which the current is very sensitively dependent on $D$. Small changes to this parameter can result in drastic changes to both the magnitude and direction of the current. (In fact, if we choose an even finer step-size for $D$ we find that it is even more sensitive).

For small $D$ values we see a strong positive current. This is because particles feel little-to-no effect when entering the interaction region and pass straight through relatively unscathed. As $D$ increases, there is a gradual decrease in the current until $D \approx 0.561$ where there is a sharp decline in the current (see inset of Fig. 2.5). After this $D$ value the magnitude and direction of the current oscillates erratically until $D \approx 0.5756$. That is, as the coupling parameter $D$ is varied, the current, originally in one direction, can drop to zero and then reverses. In the forthcoming we associate the frequent current reversals to the underlying transient chaotic dynamics. For $D \gtrsim 0.5756$ the current plateaus and finally at $D \approx 0.58$ the current makes a sharp rise, becoming positive, before tending to zero. This sharp rise can be understood if we look at the interaction potential. As mentioned in § 2.1, when $D$ increases so does the energy contained in the interaction potential and consequently particle $A$ initially has less energy. More concretely, as $D \to (0.9 - 1/\pi \approx 0.5817)$ then $E_1 \to 1/\pi \approx 0.3142$ (barrier height of the washboard potential). Therefore, particle $A$ will have sufficient energy to make it over the potential barriers and thus mount
2.2. PARTICLE CURRENT

Figure 2.5: The current as a function of $D$. The inset displays the current for the full range of $D$ values, namely $0 \leq D \lesssim 0.5817$. The main figure displays, in detail, the sensitivity of the current to changes in $D$. This corresponds to the bottom right corner of the inset.

an independent escape. However, as it is approaching the interaction region, it must share energy with particle $B$ and therefore large distances $|q - Q|$ are highly unlikely as neither particle will have sufficient energy to make it over the barriers of the washboard potential. This is clarified in the next section.

Another interesting feature of this plot is the numerous plateaus that can be seen for negative values of the current. It appears that there are certain ranges of $D$ where the current does not oscillate erratically, but rather, it stays almost constant. This indicates that in these windows the current is stable with respect to small changes of the coupling strength.


2.3 Restrictions on the Coupling Strength

The interaction potential considered here allows for the effective decoupling of the particles. This can happen in two ways. The first is that the distance between the particles becomes large resulting in a very weak particle interaction. The second way in which the particles can effectively decouple is through complete synchronisation. Here the interaction between the particles completely ceases. This case is considered in § 2.5. Thus a number of transport scenarios are possible. The particles can undergo independent motions: either, a single particle travels through the potential landscape (the other remaining trapped), or both particles are transporting. Alternatively, the particles can travel through this landscape in close proximity continuously exchanging energy (this includes the possibility of complete synchronisation where there is no energy exchange). The coupling strength determines which of these scenarios are possible. These ideas are captured in the following theorem and subsequent discussion.

**Theorem 2.1.** For systems of the form Eq. (I.1) containing at least one open component $U(q)$ – the washboard potential – providing the minimum barrier height, and interaction potential $H_{\text{int}}$, defined in Eq. (I.3) and Eq. (I.4) respectively, single particle directed transport is possible only for values of the coupling strength satisfying

$$D < E - 1/\pi,$$

where $D$ is the coupling parameter and $E$ is the system’s energy.

**Proof.** Let $Q$ be the spatial coordinate of the additional oscillator, and $P$ its momentum. Assume that the relative distance $d = |q - Q|$ is increasing with one particle trapped in a potential well. Without loss of generality we can take the particle with coordinate $q$ to be the transporting particle in a washboard potential and $Q$ the coordinate of the trapped particle. It is sufficient to consider the ideal situation where $Q = P = 0$, i.e. when the system’s energy is shared between the transporting particle
and the interaction potential. This set-up ensures that the transporting particle only has to overcome potential barriers in the $q$ direction. The effect of $Q, P \neq 0$ is to further restrict the range of $D$ for which the inequality Eq. (2.9) holds true.

Now consider the interaction and washboard potentials. As $|q - Q| \to \infty$ then $H_{\text{int}} \to D$. The potential energy for the barriers of the washboard potential is $E_b = 1/\pi$. Thus, for transport to occur, the following must be satisfied

$$E > 1/\pi + D.$$  \hbox{(2.10)}

Rearranging this we obtain

$$D < E - 1/\pi,$$  \hbox{(2.11)}

which concludes the proof.

\hfill ☐

**Corollary 2.1.** For Model One with system energy $E = 0.9$ and initial conditions as described in §2.1, with one particle approaching a second stationary particle, the transporting particle is unable to leave its starting potential well, and thus reach the interaction region, for $D > D_c$ where $D_c = 0.9 - 1/\pi$ ($\approx 0.5817$).

**Proof.** The proof follows directly from Theorem 2.1.

\hfill ☐

It is important to note that Theorem 2.1 says little about the properties of the potential function $V(Q)$. The only restrictions placed on $V(Q)$ thus far is that it is a positive semi-definite function (see Eq. (1.1)), and that it has a minimum barrier height that is at least that of $U(q)$ (i.e. $\geq 1/\pi$). Further, the possibility of two-particle transport has not been considered. The following discussion will consider the case of two-particle transport when both $U(q)$ and $V(Q)$ are washboard potentials (Model One).
For both particles to escape independently requires each particle to have a minimum energy of $E_m = E_b = 1/\pi$ (washboard barrier height). Assuming sufficient distance between the particles such that $H_{\text{int}} \approx D$, a restriction is placed on the coupling strength $D$ as

$$E = 0.9 \geq D + 2E_m = D + 2/\pi,$$

Rearranging reveals that

$$D \leq 0.9 - 2/\pi = D_2 (\approx 0.263).$$

Thus independent directed transport for two particles is possible only for $D \lesssim D_2$. However, it is expected that a significant period of transient chaos is required such that a suitable transfer of energy between the particles takes place, i.e. one that sees particle $B$ attain enough energy to overcome the washboard barrier height $E_b$. Importantly, for $D \lesssim D_2$ the duration of transient chaos is expected to be close to zero, due to the weak interaction, hampering any significant transfer of energy between the particles.

Turning to transport that is achieved by means of cooperation between the particles where $D > D_2$, simulations reveal that when the particles are close together (but not synchronised) the dynamics is chaotic. In this situation the particles cannot organise themselves such that a coherent energy exchange takes place allowing the particles to cooperatively overcome successive potential barriers and undergo permanent directed transport. Rather, the chaotic energy exchange seems to favour an optimal energy fluctuation that ejects one particle from the interaction region at the expense of the other.
2.4 Phase-Space Dynamics

In § 2.1 we illustrated some qualitatively different transport scenarios that are present in the system. As a further illustration of the phase-space dynamics, we present here a method that illuminates the dynamics of each particle, using various values of $D$. Trajectories, evolving in the four dimensional phase-space on the three dimensional energy hypersurface can be represented by examining the following surfaces

$$\Sigma_1 = \{q, p \mid U(Q) = 0\}, \quad (2.12)$$

and

$$\Sigma_2 = \{Q, P \mid U(q) = 0\}, \quad (2.13)$$

where the surface of section $\Sigma_1$ will show the dynamics of particle $A$, and $\Sigma_2$ that of particle $B$, respectively. As an explanation for the choice of surfaces, note that the coordinates $q, Q$ are unbounded and, in addition, the escape of either particle is not excluded. Further, the escape of a particle can proceed with positive or negative momentum and thus a typical Poincaré section (with fixed sign of the momentum) is not suitable here.

Returning again to the table of $D$ values above, Fig. 2.6 shows the surfaces of section for $D = 0.3$, $D = 0.5672$, and $D = 0.58169$ (from top to bottom with increasing size of $D$, and $\Sigma_1$ on the left and $\Sigma_2$ on the right). Note that for both surfaces, the coordinates $q$ and $Q$ in Fig. 2.6 are shown mod(1). We see that for a fairly low value, $D = 0.3$, exclusively regular motion occurs. Importantly, particle $A$ always maintains a strong positive momentum characterised by the densely covered curves associated with rotational motion, while particle $B$’s motion is bounded with it undergoing small oscillations about its starting position. With this $D$ value, particle $B$ contributes nothing to the net current. However, with the significant contribution
from particles $A$, with all trajectories evolving in the range of positive velocities, we can expect a strong positive current. Increasing the coupling strength to $D = 0.5672$ we see much more interesting and complex behaviour in phase-space. In particular, many of the particles initially at rest escape from their starting potential well. This escape happens after a chaotic transient which sees particle $B$ gaining enough energy to escape. On the surfaces $\Sigma_1$ and $\Sigma_2$ this motion is characterised by scattered points (representing the chaotic transient) and densely covered curves (representing the rotational motion that ensues after a particle has escaped). Further, as there is only sufficient energy for one particle to escape, the remaining particle becomes trapped, and oscillates around the bottom of a potential well. This can be seen on the surfaces as the elliptic type curves occupying the centre of these figures. There do, however, remian particles that stay trapped from the beginning in their starting potential well. Zooming in on the central region of this figure, reveals that there is indeed regular dynamics present in the system. In addition, there is also chaotic motion for some of the particles. This corresponds to the chaotic transient that both particles experience before one escapes. Furthermore, as was seen in § 2.1, it is possible for particle $B$ to escape. This is reinforced by Fig. 2.3d.

Finally, for a strong coupling $D = 0.58169$ both surfaces are largely covered by scattered points (bottom panels). This indicates that the motion of the particles is highly chaotic. There does appear to be some transport in the dynamics, but this has a possible explanation. As can be seen in Fig. 2.3e both particles can travel large distances in a relatively short time, in interludes of rotational motion where the particles stick to ballistic-like channels, but afterwards become once again trapped in potential wells for some time (this is discussed in more detail in § 2.5). However the particles do return to full chaotic motion after this transient of almost regular motion. Further, with respect to the lines $p = 0$ and $P = 0$, the surfaces appear to be symmetric. This indicates that an ensemble of particles contribute nothing to the net current.
Figure 2.6: Surfaces displaying the phase-space dynamics of particle $A$ (panels on the left) and particle $B$ (panels on the right) for 3 different $D$ values. From top to bottom these are $D = 0.3$, $D = 0.5672$, and $D = 0.58169$. The coordinates $q$ and $Q$ are presented mod(1).
2.5 Dynamical Decoupling

There exists the possibility that for any value of the coupling strength $D$ the particles will completely synchronise, and thus effectively decouple, in a process that will be called dynamical decoupling. When this process occurs the system’s energy is split evenly among the two subsystems, leaving no energy in the interaction potential. It would appear that dynamical decoupling is possible only in systems where the underlying subsystems are the same. In Model One, for example, both subsystems are washboard potentials. In contrast, Model Two (see § 3.1) has two different underlying subsystems and therefore dynamical decoupling seems unlikely unless the units are rigidly coupled.

Turning to Model One, complete synchronisation reduces this system to two identical pendula defined by

$$\ddot{q} = -\sin(2\pi q) \quad \text{&} \quad \ddot{Q} = -\sin(2\pi Q). \quad (2.14)$$

Now the dynamics are completely integrable. Motion takes place on a two-dimensional surface in the four-dimensional phase-space. For transport to occur in this case, all that is required is that the subsystem’s energy exceeds the washboard barrier height $E_b = 1/\pi$, meaning the system’s energy must satisfy $E > 2/\pi$.

Importantly, it is expected that dynamical decoupling only happens in the range of extremely strong coupling and therefore is not present in Model One for the particular initial conditions (including the system’s energy – cf. § 2.1) chosen for the numerics. However, the effects of dynamical decoupling can be seen, for relatively low coupling strengths, in the form of ballistic-like channels which appear when the particles are close to one another and the interaction between them almost vanishes; that is $q \approx Q$. When these conditions are met, the particles can travel in a directed fashion for significant amounts of time. An example of this can be seen in Fig. 2.3e where the particles travel in the range of negative $q_{1,2}$ for $t > 500$ time units, before settling back
into chaotic motion. This is reminiscent of studies by Yevtushenko et al. (2000), etc (for more see § 1.5.1), where similar effects can be observed. However, the mechanisms that create these ballistic channels are not the same. The channels present in their study requires a mixed phase-space. In contrast, the ballistic channels observed in Model One are induced by closeness of the particles. Importantly though, the effects are similar — finite periods of directed transport, followed by a chaotic interval of diffusive motion.

With regard to the emergence of a current, the ballistic channels present in Model One do not appear to be of much consequence when averages over time and ensemble are considered. For ballistic channels in a mixed phase-space, born out of ‘stickiness’ to regular island, the converse is quite often true. Due to a lowering, or indeed a breaking, of some symmetry in these systems the ballistic channels contribute with different weights to the net current. Therefore, a non-zero net current often results. In Model One, however, there can exist only two of the above mentioned ballistic channels where $q \approx Q$. In one, the particles move with positive momentum, and in the other they move with negative momentum. The respective weights of these ballistic channels must be equal due to the reflection symmetry of the two washboard potentials and the interaction potential. If a non-zero net current does result in this system it is because of particle separation, and an increasing distance between the particles, rather than the particles evolving in an almost synchronous manner for finite times. The asymmetry here, with respect to the non-zero net current, is induced by the choice of initial conditions and will be discussed in detail in Chapter 3.

2.6 Manifestations of Chaos

With regard to transport, the presence of chaos is of critical importance. It is chaos that serves to break up separatrices that separate regions of bounded and unbounded
motion thus allowing particles to explore wider regions of phase-space. However, unless the chaos is transient in nature, it is very likely that the dimer will move erratically with many changes of direction that will render directed transport impossible. For systems of coupled oscillators there are numerous indicators that can be used to gauge the prominence of transient chaos in the system. Two of these are discussed now.

2.6.1 Particles Sojourn in Interaction Region

A more direct way of examining the effect that the coupling strength has on the particles is to calculate the amount of time that particles $A$ and $B$ spend in the interaction region — the region where the particles interact chaotically. More formally, the time interval (sojourn) for which the particles satisfy the condition

$$|q(t) - Q(t)| \leq 10,$$  \hspace{1cm} (2.15)

has been calculated. When the distance $|q(t) - Q(t)| > 10$, the gradient of the interaction potential will almost be equal to zero, and the energy exchange between the particles will be neglible.

Figure. 2.7 (left panel) shows the sojourn times for an ensemble of initial conditions corresponding to $D = 0.5617$ and $D = 0.5672$ as a function of the angle $\alpha = \tan^{-1}(p(0)/q(0))$, which can be viewed as the incident angle in the $(q,p)$ phase plane of the initially free particle $A$. We see that with the lower $D$ value (red dots in figure) the particles all spend a relatively short time in the interaction region and that the time corresponding to each initial condition is almost the same. Associated with this is a fairly large current, $\bar{p} = 0.262$ (cf. Eq. (2.5)), indicating that the particles leave the interaction region in a preferred direction. In contrast, for the second $D$ value (green dots in figure) the time for each initial condition is noticeably
longer than in the previous case. Further, these times are much more varied and there is a large difference between the smallest and greatest time for this ensemble (approximately 2700 time units). That is, as a hallmark of chaotic scattering (Bleher et al., 1988, 1990; Ott, 1992; Tél & Gruiz, 2006; Tél, 1990); the sojourn time depends sensitively on changes of the initial values because chaotic saddles, formed by the intersecting stable and unstable manifolds of unstable periodic orbits, govern the dynamics. In more detail, escaping trajectories follow the unstable manifolds of saddle points, whereas there are trajectories that remain in the interaction region, or spend at least some time there, before escape as a consequence of the presence of chaotic saddles. From the corresponding small value of the current, $\bar{p} = 0.009$ (cf. Eq. (2.5)), we infer that the exit of the particles from the interaction region proceeds such that they virtually balance each others contribution to the net current. The window containing no points is due to the fact that with a lower $D$ value the range of momenta taken initially by an ensemble of particles $A$ is smaller than the range for a larger $D$ value. This is clearly seen in the example initial conditions shown in Fig. 2.2.

Finally in the case that $D = 0.58169$ (Fig. 2.7 - right panel), corresponding to a vanishingly small current, we see all of the particles spend the entire duration of the simulation in the interaction region (50,000 time units). This is a possible mechanism that allows for the reduced current that can be seen.

### 2.6.2 Energy Redistribution Processes

In order to gain more insight into the dynamics of the system a further statistical analysis, going beyond the consideration of individual trajectories (cf. § 2.1), is carried out. Previously we have looked at the partial energies for particles $A$ and $B$ at the end of a simulation, using example trajectories (discussed in § 2.1). Now we will make use of histograms displaying the distribution of particle energies, using an ensemble of $N = 10^3$ initial conditions, at the end of the simulation time $T_s = 10^5$. 
2.6. MANIFESTATIONS OF CHAOS

Figure 2.7: Sojourn time of an ensemble of particles in the interaction region, versus the incident angle $\alpha = \tan^{-1}(p(0)/q(0))$. Left: The blue (scattered) points show the time for the ensemble when $D = 0.5672$. Similarly, red (lower line) is for the particles when $D = 0.5617$. Right: Same as left with $D = 0.58169$.

For continuity, we will examine the histograms corresponding to the five $D$ values used earlier in § 2.1.

In Fig. 2.8a ($D = 0.3$) we see that at the end of the simulation it is particle $A$ (red in figure), for the entire ensemble, that possesses the majority of the energy in the system. While particle $B$ (blue in figure) does possess some energy, it is not sufficient for it to escape from its starting potential well. Since the energy of particle $B$ is below the energy of the confining centre-saddle points, escape of particle $B$ over the barriers is prevented. A more detailed consideration of the potential landscape will be presented in Chapter 4.

We see a similar histogram in Fig. 2.8b ($D = 0.5613$). The difference this time is that particle $A$ has sacrificed some of its energy to particle $B$. This is not unexpected if we consider the example trajectory shown in Fig. 2.3b, where the interaction with particle $B$ has a significant impact on the trajectory of particle $A$.

Again in Fig. 2.8c (with $D = 0.5617$) we have a similar histogram as seen in
Fig. 2.8a and Fig. 2.8b with a further loss in energy for particle \( A \), and a gain for particle \( B \), and thus the final particle energies lie closer together. A slightly more intriguing histogram is presented in Fig. 2.8d \((D = 0.5672)\). This \( D \) value corresponds to that of Fig. 2.3d where it is particle \( B \) not particle \( A \) that escapes. Consequently, the histograms shows that indeed, there are some particles \( B \) that possess the majority of the energy at the end of the simulation. However, it is clear that for the ensemble, the majority of particles that contain most of the energy are in fact particle \( A \).

Finally, in Fig. 2.8e \((D = 0.58169)\) we see that there is a large distribution in the final energies of each particle, with no obvious bias favouring the partial energy of either particle.

These histograms for the various \( D \) values, do not give a full indication of what the current will be for those respective \( D \) values. They do however allow us to make assumptions. For example, Fig. 2.8a shows that particles \( A \) contain almost all of the energy at the end of the simulation. We therefore expect that particle \( A \), for the entire ensemble, will make a large contribution to the net current. Further, if we were naively to include the corresponding example trajectory (Fig. 2.3a) in our assumption, we might conclude that there will be a large positive net current for the ensemble.

Taking the next \( D \) value and making similar assumptions to those above, one might conclude that again there is a large positive net current. This time however, the current would not be quite as strong, as the final energies for the ensemble indicate that particle \( A \) has sacrificed energy to particle \( B \).

The same applies for the final \( D \) value, where one might conclude that, because of the spread of energies for both particles, the current will be quite small.
Figure 2.8: Histograms displaying the final partial energies, again using the five \( D \) values from the table in § 2.1, of particles \( A \) (red) and \( B \) (blue) for an ensemble of initial conditions.
2.7 Chapter Summary

The conservative dynamics for systems of coupled particles have been explored through the study of Model One which consists of two washboard potentials that are coupled via an interaction potential. This proves to be a rich source for complex dynamics which produces numerous interesting results. For example, with fine tuning of the system’s parameter regulating coupling strength, particle scattering leading to the emergence of a non-zero net current, or bond formation (dimerisation) yielding a zero net current, are possible outcomes in this model. Moreover, it has been demonstrated that this system is extremely sensitive with respect to small changes in this parameter in that multiple current reversals are observed in a small range of values of this parameter. Reasons for this sensitivity will be explored in Chapter 4.

A novel aspect of these autonomous Hamiltonian systems is that directed transport, when it occurs, is regular and permanent. Chaos is needed only in an initial phase of the dynamics to guide trajectories beyond separatrices into the range of unbounded motion. This contrasts with the transport observed in non-autonomous Hamiltonian systems where there is a mixed phase-space (Denisov & Flach, 2001). In these non-autonomous systems, finite bursts of almost regular transport are separated by periods of chaotic motion. Thus the autonomous systems, where directed transport is provided solely by regular motion, appear to be favourable with respect to directed transport. However, it should also be mentioned that the transport observed in the autonomous case is quite often a cooperative effect relying on a favourable energy exchange between subsystems.

An interesting observation is that according to the theory of time-reversal symmetry, Model One should produce a zero net current for all values of \( D \). The explanation of why Model One, and systems like Model One, can still produce a directed current is the subject of Chapter 3. This chapter looks at time-reversal symmetry for the class of systems whose equations of motion are given by Eq. (I.2) (of which Model One is
a member). It will be explained in detail how this symmetry is broken in practice, thus allowing for the emergence of a non-vanishing net current. Further, a second model will be introduced that is similar to Model One with the exception that one of the washboard potentials is replaced by a different potential. This new potential serves to break one of the spatial symmetries of the system. The consequences of this broken symmetry will also be examined.
CHAPTER 3

Symmetry Considerations

In systems that satisfy certain spatial and temporal symmetries it is possible to find, in phase-space, two trajectories that nullify each others contribution to the net current. That is to say, for each trajectory in phase-space there exists another complementary trajectory such that collectively both trajectories produce zero net current. Therefore, if a system is to express a non-zero net current, some of these symmetries must be broken. Quite often this is achieved through the addition of a periodic (but non-symmetric) time dependent drive to the system (Denisov et al., 2002a). Analogously, in the autonomous case the introduction of a static bias force that penetrates the plane of motion, usually suffices when breaking the spatial symmetry thus allowing for the emergence of a non-zero current (Speer et al., 2007b).

This chapter will look at a mechanism that serves to break the spatio-temporal symmetries and thus allow for the possible occurrence of a non-zero current. The focus is on autonomous systems modelling the interaction of coupled particles. Crucially, in systems (with a mixed phase-space) that rely on regular interludes between periods of chaotic motion for directed transport, the chaotic periods are seen as destructive with regard to directed transport, in that the average velocity of trajectories in the chaotic component of phase-space will be close to zero. In contrast, the systems looked at here require chaos in an initial stage of the dynamics so that trajectories can be captured by hyperbolic structures allowing them to escape. The emergence of
a non-zero net current is still dependent on other factors. Particular attention will be given to the symmetry properties induced by the inclusion of an interaction potential.

The symmetry properties derived will be illustrated via an example model system. This model is introduced now.

3.1 Spatially Asymmetric Model (Model Two)

Model One was idealised in that both coordinates of the system obeyed a spatial symmetry; namely the system remains invariant under a change of sign of both coordinates. This is not true of Model Two were a new potential is introduced that has the effect of breaking a spatial symmetry for one of these two subsystems. Rather than having two particles each evolve in a washboard potential, as in Model One, in this model only one particle will evolve in a washboard potential. This particle will be coupled to a second particle (which is unable to contribute to the net current due to energy constraints) that will serve as an energy deposit from which the particle evolving in the washboard potential can draw energy. The second potential is an anharmonic oscillator and interactions with this oscillator are local in nature due to the type of interaction potential and the finite amount of energy injected into the system. It is defined by

\[ V(Q) = \exp(-Q) + Q - 1. \] (3.1)

Unlike the washboard potential which has bounded potential energy \( U(q) \leq E_b = 1/\pi \), this anharmonic oscillator has unbounded potential energy for \( \pm Q \); i.e \( V(Q) \to \infty \) as \( Q \to \pm \infty \). Note the asymmetry of this potential, i.e. \( V(Q) \neq V(-Q) \), as this will be important when the symmetry properties of this model are discussed. Before moving on to the main focus of this chapter it is worthwhile exploring some of the coupled system dynamics. The equations of motion are
\[ \ddot{q} = -\sin(2\pi q) - D \left[ \frac{\tanh(q - Q)}{\cosh(q - Q)} \right] , \quad (3.2) \]

\[ \ddot{Q} = \exp(-Q) - 1 + D \left[ \frac{\tanh(q - Q)}{\cosh(q - Q)} \right] . \quad (3.3) \]

Let us assume finite system energy. For \( D = 0 \), the system decouples into two integrable subsystems and the dynamics is characterised by individual regular motions of the particle in the washboard potential, and bounded oscillations of the additional degree-of-freedom (due to the energetic constraints), respectively. For \( D \neq 0 \), the subsystems interact, exchanging energy. While the \( Q \)-oscillator performs solely bounded motion there is the possibility that, for an escaping particle, the corresponding coordinate, \( |q| \), attains large values and thus the related interaction forces, \( \partial H_{\text{int}} / \partial q \) and \( \partial H_{\text{int}} / \partial Q \), vanish asymptotically, allowing transient chaos (Zaslavsky, 1985, 1998; Ott, 1992). That is, for large distance \( |q - Q| \gg 1 \), the interaction vanishes with the result that the two degrees-of-freedom decouple, rendering the dynamics regular (see also § 2.1).

Looking at example trajectories for three representative coupling values reveals some of the system’s dynamics. Fig. 3.1 presents the time evolution of the coordinates \( q \) & \( Q \) for \( D = 0.4 \) (top row), \( D = 0.75 \) (middle row), and \( D = 1.5 \) (bottom row). In addition, the corresponding partial energies of the particle and the deposit degree-of-freedom are presented. The partial energies for both particles are given by

\[ E_q = \frac{1}{2} \dot{q}^2 + U(q) + \frac{1}{2} H_{\text{int}}(q, Q), \quad E_Q = \frac{1}{2} \dot{Q}^2 + V(Q) + \frac{1}{2} H_{\text{int}}(q, Q), \quad (3.4) \]

where the interaction energy has been evenly divided between the two particles. Details of the initial conditions are given in § 3.3.

Three qualitatively different transport scenarios are presented. Note that for the numerics the system’s energy is fixed at \( E = 1.5 \). Further, the initial conditions
Figure 3.1: Time evolution of the coordinates $q$ (solid blue line) and $Q$ (dashed red line) for three different values of the coupling strength $D$: (a) $D = 0.4$, (b) $D = 0.75$, and (c) $D = 1.5$. 
have been chosen so that all the system’s energy is initially in the deposit degree-of-freedom. For the low value $D = 0.4$ (top row) the washboard particle undergoes small amplitude oscillations about a potential minimum. Crucially, with regard to transport, these oscillations are much lower than the barrier height $E_b = 1/\pi$ of the washboard potential. In contrast, the deposit degree-of-freedom sees oscillations of much larger magnitude. Looking at the partial energies of the washboard particle and the anharmonic oscillator, it can be seen that there is an insufficient energy exchange to allow for the washboard particle to overcome the barrier height $E_b$ – a prerequisite for the occurrence of transport. The dynamics changes drastically when the coupling strength is increased to $D = 0.75$ (middle row). The early dynamics ($t < 10$) is similar to the situation described above. Subsequently, the washboard particle escapes from its starting potential well and travels to multiple wells in both directions. At $t \approx 40$ the washboard particle gains sufficient energy to allow it to undergo independent directed transport. That is, after a chaotic transient, the two subsystems decouple rendering the dynamics regular. The chaotic exchange of energy preceding the directed transport of the washboard particle is clearly visible in Fig. 3.1.

It is also clear that after the chaotic transient, the energy exchange between the two oscillators terminates. A further increase in the coupling strength to $D = 1.5$ (bottom row) results in a third qualitatively different transport scenario. It appears that the washboard particle is free to travel multiple potential wells. However, for the duration of the simulation it is confined to potential wells in the range $-2.5 < q < 2.5$. The reasons for this are two-fold. Firstly, by Theorem 2.1 with $D = 1.5$ (and $E = 1.5$) the possibility of directed transport for the washboard particle is excluded. Secondly, the system’s (finite) energy means that oscillations of the anharmonic potential are bounded. Combined, this results in two oscillators that remain in close contact and under constant chaotic energy exchange.
3.2 Symmetry Breaking

It was shown that with a suitable choice of parameters Model Two can exhibit directed transport, which is a necessary, but not sufficient, condition for a system to show a non-zero net current. However, the class of systems that Model Two belongs to has time-reversibility symmetry and the implications of this with regard to the net current are extremely important. These implications, and a mechanism for destroying this symmetry, will be the focus of this section.

The class of systems in question are Hamiltonian and of the form

$$H(p, q) = \frac{1}{2}p^2 + U_{\text{eff}}(q) \quad (3.5)$$

where $p, q \in \mathbb{R}^n$, $p$ and $q$ are the canonically conjugated momenta and positions, and $U_{\text{eff}}(q)$ is the potential function. With transport and directed current being of interest, it will be assumed that $U_{\text{eff}}(q)$ provides an open component. To reiterate, this means that on constant energy surfaces, the system may be unbounded in one, or more, of its coordinates.

The corresponding Hamiltonian equations $\dot{p}_i = -\partial H/\partial q_i$ and $\dot{q}_i = \partial H/\partial p_i$, $1 \leq i \leq n$, exhibit the time-reversibility symmetry, i.e. there exists a time-reversal operator $\hat{\tau}$ such that if $X$ is a solution, then so is $\hat{\tau}X$. In more detail, suppose that solutions take the form $X(t) = [p(t), q(t)]$. Applying the time-reversal operator yields $\hat{\tau}[p(t), q(t)] = [-p(-t), q(-t)]$. This operation is involutory as $\hat{\tau}^2[p(t), q(t)] = [p(t), q(t)]$. As for the implication of time-reversibility with respect to the net current, consider a solution with initial condition (at $t = 0$) given as $X(0)$. Given a finite observation time $T$ (relevant for numerical and experimental studies), let $X(t)$ evolve from $X(0)$ to $X(T)$. This trajectory will be called the forward trajectory. At this point the time-reversal operator is applied which switches the sign of the momenta and changes the direction of time. This creates a new initial condition $\hat{\tau}X(T)$ which can be evolved in (negative) time. This trajectory will be called the backward tra-
3.2. SYMMETRY BREAKING

jectory. In fact, when the system is evolved from this new initial condition it traces over the forward trajectory in coordinate-space. Note that the forward and backward trajectories coincide in coordinate-space, but not in phase-space due to the change in the sign of momenta. Given the general nature of the above initial condition \( X(0) \), we can conclude that on constant energy surfaces, for each such initial condition there exists a corresponding initial condition \( \tau X(T) \) such that they cancel each other’s contribution to the net current. Therefore, for systems with time-reversibility symmetry there is no preferred direction of the flow thus preventing the emergence of a directed current.

The content of the above discussion is shown schematically in Fig. 3.2. Imagine \( q = \theta \) is the angle of rotation of a pendulum, and \( p = \dot{\theta} \) is the corresponding angular velocity. Then the top half of the figure (in red) shows the phase portrait of a pendulum, with initial condition \( X(0) = (p(0), q(0)) \), undergoing rotational motion. The trajectory terminates at \( X(T) = (p(T), q(T)) \). The bottom half of the figure (in blue) is the time-reversed counterpart of this trajectory, \( X(T - t) \), with initial condition \( \tau X(T) = (-p(T), q(T)) \). With a view to the present work, we can imagine a single particle, with position \( q \) and momentum \( p \), undergoing rotational motion in a washboard potential.

In the literature it is common to apply the time-reversal operator to the system and the original initial condition \( X(0) \) (Lamb & Roberts, 1998). Indeed, this produces another possible motion of the system. However, it is not always the case that these two trajectories produce average velocities that are equal in magnitude but opposite in sign. For example, it is possible to envisage a potential such that a particle moving to the right will fall into a ‘trap’, while the particle moving to the left will experience unbounded motion. Clearly, the sum of the two average velocities will not equal zero. The point emerges that to produce (and guarantee that) two trajectories with zero average velocity, the first needs to be evolved to some terminal time \( t = T \) at which point the time reversal operator is applied.
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**Figure 3.2:** Schematic illustration of the forward (red) and backward (blue) trajectories for a particle in the regime of rotational motion. The forward trajectory has initial condition \( X(0) \) and terminal coordinate \( X(T) \), whereas the time-reversed trajectory has initial condition \( \tau X(T) \) and terminal coordinate \( \tau X(0) \).

It should also be mentioned that the act of selecting an initial condition can be sufficient in itself to violate time-reversibility symmetry. That is, even though the equations of motion are time-reversal symmetric, not all solutions need necessarily have this symmetry. This is the case for trajectories where the initial condition and its time reversed counterpart follow distinct paths in phase-space. As an example of such a trajectory consider a continuously rotating pendulum (cf. Fig. 3.2). So by creating a trajectory with time-averaged velocity \( \nu \neq 0 \), over an observation time of duration \( t = T \), and initial condition \( X_0 \), time-reversibility symmetry has been broken, unless a second initial condition \( \hat{\tau} X_T \) is chosen that produces a trajectory with time-averaged velocity \( -\nu \). This is not true for self-reversed trajectories where
the initial conditions $X_0$ and $\dot{X}_T$ produce trajectories that coincide in phase-space. The librating trajectories of a pendulum are self-reversed. See Fig. 3.3 for a schematic illustration of this. The same principles apply to trajectories that wander chaotically in phase-space.

Given what has just been discussed, it seems a rather hopeless situation to find Hamiltonian of the form given in Eq. (3.5) that expresses a non-zero net current, because every initial condition is related to another that negates its contribution to the current. This statement is true as long the entire energy surface is populated with initial conditions. However, for systems with an open component, i.e. unbounded in at least one of its coordinates, it is infeasible to populate an entire energy surface with initial conditions. Therefore, it is more natural to define a finite set of initial conditions which, given the infinite extent of (at least one of) the coordinates can
be regarded as *localised in space*. Such sets of initial conditions are frequently used in applications (see Hennig et al. (2011a) for an example), and are chosen to be physically relevant, such as for the problem of a particle flow emerging when the particles are initially trapped in a single well of a spatially infinitely extended multiple well potential. Indeed this will be done when Model Two is further examined in a later section.

Looking more closely at the implication of choosing localised initial conditions, it is supposed that the coordinates are localised in the domain $q_{j,l} \leq q_j(0) \leq q_{j,r}$ with $1 \leq j \leq n$ representing the index of each degree-of-freedom (which for the present discussion is not restricted to two), and the subscripts $l$ and $r$ denote left and right respectively. Let a trajectory (with regard to a finite observation time $T$) be *transporting* if (i) at least one of the coordinates $q_j(t)$ escapes from the domain of the localised initial conditions in some time $0 < t_{\text{escape}} \ll T$ and (ii) it subsequently undergoes directed motion, that is, $\langle p_j(t) \rangle \neq 0$ for $t_{\text{escape}} \leq t \leq T$ where $\langle \cdot \rangle$ denotes the average with respect to time. This gives a trajectory moving away from the set of localised initial conditions such that at the end of the observation time one of the terminal coordinates obeys $q_j(T) < q_{j,l}$ or $q_j(T) > q_{j,r}$ for some $j$. Thus, the situation has arisen where the initial condition of the corresponding backward trajectory, which would compensate the contribution of the forward trajectory to the current, is not contained in the set of localised initial conditions. This seems to suggests that in systems where time-reversibility has been broken, via the use of localised initial conditions, there will be a non-zero directed current. This is not necessarily the case. In fact other symmetries need first to be violated, i.e. spatial symmetries. This will be seen more clearly when the symmetry properties of Model Two are considered. First, let us examine the conditions that allow for the occurrence of a non-zero current in Model One.
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3.2.1 The Emergence of a Non-Zero Current in Model One

Before moving on, let us return to Model One to examine the initial conditions used there. It is worth noting that as the system is spatially symmetric and yet a non-zero current can emerge in the ensemble dynamics, the choice of initial conditions must be extremely important. First, let us recall what these initial conditions are. Let us denote some initial condition by \( X(0) \) where \( X(0) = (p(0), q(0), P(0), Q(0)) \) with \( Q(0) = P(0) = 0, p(0) > 0 \) and \( q(0) \in (-25.5, -24.5) \). Thus the early dynamics will see the coordinate \( q(0) \) approach \( Q(0) \). For the actual current output, as a function of the coupling strength \( D \), see Fig. 2.5.

Applying the time-reversal operator to \( X(0) \) yields \( \tau X(0) = \hat{X}(0) = (-p(0), q(0), 0, 0) \). The flow, generated by the equations of motion with initial conditions \( X(0) \) and \( \hat{X}(0) \), do not necessarily produce zero-averaging counterpropagating trajectories. This is clear when one considers that with \( X(0) \) the coordinate \( q(0) \) will approach \( Q(0) \). However, under the flow with initial condition \( \hat{X}(0) \) the distance between these coordinates is monotonically increasing. This is true for all such initial conditions defined above. Thus, the presence of the interaction potential breaks time-reversibility for this set of initial conditions. This echoes Loschmidt’s paradox in that the underlying system obeys time-reversibility, yet some ensembles do not obey the symmetry. Thus, this system has helped to illuminate an important point, from the point of view of current generation. Namely, a system (with initial condition \( X(0) \)) under time-reversal does not necessarily produce counterpropagating trajectories, \( X(0) \& \tau X(0) \), that combined have zero averaged current.

In fact, the appropriate initial condition \( \hat{X}(0) \) that would produce the counterpropagating trajectory negating the current contribution of the trajectory with initial condition \( X(0) \) is given by \( \hat{X}(0) = (-p(0), -q(0), 0, 0) \). Crucially, the set of initial conditions described above does not contain \( \hat{X}(0) \), and thus this explains the emergence of a current. It should be noted that \( \hat{X}(0) \) is not created through any time-reversal operation. Rather, this initial condition is generated from the system’s
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Spatial symmetries. Another point to note is that if the original initial conditions \( X(0) \) are evolved for any time \( T > 10 \) (which the simulations exceed by far) then the time-reversed initial condition \( \tau X(T) \) is outside the set of localised initial conditions (as described above). Thus the temporal and spatial symmetries have been violated through the choice of initial conditions.

3.2.2 Time-Reversal Symmetry Manifolds

For Hamiltonian systems of the form Eq. (3.5) time-reversibility is manifested in coordinate-space in the symmetry features induced by reflections on the time-reversibility symmetry manifolds. In the case of Models 1 & 2, or any two-degree-of-freedom system for that matter, the symmetry manifolds are represented by symmetry lines. In general, for n-degree-of-freedom systems, these symmetry manifolds are obtained by setting the velocities (momenta) equal to zero. This produces an n-dimensional ‘mirror’ plane

\[
M = \{ q \mid p = 0 \} \quad q, p \in \mathbb{R}^n
\]  

(3.6)

where trajectories starting on this plane will follow the same path in coordinate-space in forward and backward time. More accurately, the time reversibility manifolds are given by

\[
S_k : -\frac{\partial U}{\partial q_k} = F_k(q) = 0, \quad 1 \leq k \leq n.
\]  

(3.7)

Reflections on the n symmetry manifolds obey \( q(-t+t_0) = q(t+t_0) \) and \( p(-t+t_0) = -p(t+t_0) \) where the variable \( t_0 \) denotes the time when the time evolution is started. Let us consider reflections of a trajectory, projected onto coordinate space, on the symmetry manifolds \( S_k \) induced by the corresponding operators \( \hat{R}_k \). First note that the reflections spoken of here are not spatial reflections. Rather, these reflections map each point of a trajectory onto another, \( q \rightarrow \hat{R}_k(q) \), on equipotentials, \( U(q) = ...
$U(\prod_{k=1}^{m} \hat{R}_k(q))$, such that the sign on the right hand side of the equations of motion for $\dot{p}_k$ are reversed, $F_k(q) \rightarrow -F_k(\hat{R}_k(q))$, with $1 \leq k \leq n$. This is clear when one considers the form of the Hamiltonian being even in the momenta $p$ and the fact that the time-reversal operator changes the sign of the momenta $p \rightarrow -p$.

Observe that upon reflecting on all symmetry manifolds the relation $U(q) = U(\prod_{k=1}^{m} \hat{R}_k(q))$, $1 \leq m \leq n$ is left invariant under permutations of the reflection operators. In fact, time-reversing symmetry is in coordinate-space tantamount to invariance with respect to reflections on the symmetry manifolds. In more detail, any self-reversed trajectory, projected onto coordinate-space, repeatedly crosses every symmetry manifold $S_k$ upon which each time the sign of the corresponding force $-F_k(q) < \infty$ changes. Moreover, each crossing subsequent to the previous one occurs from the opposite direction. Thus there must be turning points for the trajectory implying bounded motion and no directed flow can arise. Notice that no assumptions with regard to the spatial symmetries of the trajectory are needed. In contrast, as transporting (unbounded) trajectories are not invariant with respect to reflections on the symmetry manifolds, preservation of time-reversing symmetry is not possible. A transporting trajectory may escape without having crossed a symmetry manifold at all. However, if it does cross then after all such crossings of a symmetry manifold, the escaping trajectory promotes directed transport. Nevertheless, reflections on the symmetry manifolds, mapping a transporting trajectory onto another transporting one, can induce spatial symmetries such that these two trajectories mutually compensate each others contribution to the net flow. Let the point $q_O$ in coordinate-space be an initial condition associated with a transporting trajectory. Reflecting in coordinate-space on the symmetry manifolds $S_k$ transforms an original point, $q_O$, into its image point, $q_I$, according to $\hat{R}_k q_O = q_{I,k}$ reversing the sign on the r.h.s. in the equations of motion for $\dot{p}_k$ according to $F_k(\hat{R}_k q_O) \rightarrow -F_k(q_{I,k})$. However, the magnitude of the gradients $F_k = \partial U/\partial q_k$ is not necessarily maintained. Reflection on all of the symmetry manifolds yields $\prod_{k=1}^{m} \hat{R}_k q_O = q_I$ and $U(q_0) = U(q_I)$, revers-
3.3 Effect of Broken Symmetries

It is useful to see how the above theory on spatio-temporal symmetries can be applied in practice, and in particular to see the effects of breaking these symmetries. For this reason, the spatio-temporal symmetry properties of Model Two are now examined. Particular attention is given to the phase-space dynamics and to current generation where the effects of broken symmetries is most clearly visible.

Model Two has an effective potential given (in short) by

\[ U_{\text{eff}}(q) = U(q) + V(Q) + H_{\text{int}}(q, Q) \]  

(3.8)

where \( U(q) \) is the washboard potential, \( V(Q) \) is the anharmonic (deposit) potential, and \( H_{\text{int}}(q, Q) \) is the interaction potential. Some properties of the washboard and interaction potentials were discussed in the introduction to Part I. However, it is worth
reiterating those that are relevant in this section. The washboard potential is of period one and observes the coordinate symmetry \( U(q) = U(-q) \). This amounts to symmetry with respect to \( q_n = n/2 \) for every integer \( n \). Likewise, the interaction potential is invariant under reflections of its argument, namely \( (q - Q) \leftrightarrow -(q - Q) \). In contrast, the deposit degree-of-freedom \( V(Q) \) does not obey such a reflection symmetry. That is, \( V(Q) \neq V(-Q) \) resulting in equations of motion (cf. Eq. (3.2) & Eq. (3.3)) that do not remain invariant under reflections in \( Q \).

Even with the anharmonic oscillator \( V(Q) \), which breaks a reflection symmetry of the system, Model Two still possesses time-reversal invariance. Thus, if the phase-space is entirely populated with initial conditions, then the system will produce a zero net current. This raises the question of what effect localised initial conditions (as described in § 3.2) has on the system’s current output.

At this point it is worthwhile describing exactly the set of initial conditions that were used in the numerical analysis of Model Two. These initial conditions were chosen such that the washboard particle was at rest at the origin, with the system’s energy initially residing in the deposit degree-of-freedom and the interaction potential. In more detail, at time \( t = 0 \), the washboard particle’s position and velocity were given by \( q(0) = \dot{q}(0) = 0 \). Thus the washboard particle begins its time evolution with zero energy. Assuming system energy \( E \), the set of initial conditions for the remaining degrees-of-freedom are chosen to populate uniformly and densely the level curve

\[
E = \frac{1}{2} \dot{Q}^2 + V(Q) + H_{\text{int}}(0,Q)
\]

in the \((Q, \dot{Q})\)-plane. This set is topologically a circle. Importantly, these initial conditions are unbiased in the velocity, i.e. \( \dot{Q} \leftrightarrow -\dot{Q} \).

Returning to the symmetry analysis we now turn our attention to the time-reversal symmetry manifolds. As this is a two-degree-of-freedom system, the symmetry manifolds will exclusively be termed symmetry lines. Setting the velocities in Eq. (3.2) &
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Eq. (3.3) equal to zero obtains

\[ S_1 : \sin(2\pi q) + D \frac{\tanh(q - Q)}{\cosh(q - Q)} = 0, \]  

\[ S_2 : \exp(-Q) - 1 + D \frac{\tanh(q - Q)}{\cosh(q - Q)} = 0. \]

The symmetry line \( S_1 \) exhibits the following symmetry:

\[ Q \rightarrow -Q, \quad \frac{n}{2} + q \rightarrow -\frac{n}{2} - q : \quad S_{1,n} \rightarrow -S_{1,-n} \]

with \( n \) labelling the branches of the symmetry line as \( S_{1,n} \). The occurrence of the multiple branches of the \( S_1 \) symmetry line can be understood by considering the symmetries of the washboard potential. In contrast, \( S_2 \) yields a single branch containing no apparent symmetries.

The two cases, coupled and uncoupled, result in markedly different dynamics. Notably, uncoupling the two subsystems produces integrable dynamics. The dynamics becomes non-integrable (chaotic) when the two subsystems are coupled. This complexity is also manifested in the symmetry lines \( S_1 \) and \( S_2 \). To see this, consider first the uncoupled case. With the coupling parameter \( D = 0 \), the equations representing the symmetry lines are simplified and solutions take the form \( q = n/2 \) for all \( n \in \mathbb{Z} \) and \( Q = 0 \). For \( D \neq 0 \) the solutions to the equations for \( S_1 \) and \( S_2 \) become more complicated. This point is illustrated in Fig. 3.4 which shows the time-reversal symmetry lines when \( D = 0.75 \). For illustration, only the branches of the symmetry line \( S_{1,n} \), with \( n = -1, 0, 1 \), related to the starting potential well are shown. The direction of flow, as determined by the sign of the forces \( -\partial U_{\text{eff}}/\partial q \) and \( -\partial U_{\text{eff}}/\partial Q \), is indicated by arrows in the different regions in the coordinate plane. Boundaries of the energetically-allowed region in coordinate-space are represented by the two lines labelled \( B_e \). Reflections of a trajectory, projected onto
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Figure 3.4: Time-reversal symmetry lines in the coordinate plane \((q, Q)\) for \(D = 0.75\). The system’s energy is \(E = 1.5\) and the energetically accessible region is bounded by the two curves indicated by \(B_e\). The dashed (red) line corresponds to the location of the initial conditions projected onto coordinate-space. Arrows indicate the direction of flow in different regions, as determined by the sign of the forces \(-\partial U_{\text{eff}}/\partial q\) and \(-\partial U_{\text{eff}}/\partial Q\).

Coordinate space, on the symmetry lines \(S_k\) are induced by the corresponding operators \(\hat{R}_k\) mapping each point on the trajectory to another one on equipotentials \(U_{\text{eff}}(q, Q) = U_{\text{eff}}(\prod_{k=1}^{2} \hat{R}_k(q, Q))\), such that the sign on the r.h.s. in the equations of motion is reversed, i.e., \(-\partial U_{\text{eff}}(q, Q)/\partial q \rightarrow \partial U_{\text{eff}}(\hat{R}_1(q, Q))/\partial q\) upon reflection on \(S_1\) and \(-\partial U_{\text{eff}}(q, Q)/\partial Q \rightarrow \partial U_{\text{eff}}(\hat{R}_2(q, Q))/\partial Q\) upon reflection on \(S_2\). However, the magnitude of the gradients \(\partial U_{\text{eff}}(q, Q)/\partial q\) and \(\partial U_{\text{eff}}(q, Q)/\partial Q\) is not necessarily maintained.

It is clear that the symmetry lines for the uncoupled and coupled system are significantly different. Coupling the two subsystems has the effect of contorting the symmetry lines. It should be stressed again that even though the time-reversal symmetry lines differ for each value of the coupling parameter, the result for the net current is the same when the energy surface is entirely populated by initial conditions. That is, when the energy surface is entirely populated by initial conditions,
the resulting current is zero regardless of the value $D$ which regulates the coupling strength.

Now the issue of localised initial conditions can be addressed. The initial conditions described above are shown, projected onto the $(q,Q)$-plane, as the red dashed line in Fig. 3.4 which shows the time-reversal symmetry lines for $D = 0.75$. Notice that one branch of the symmetry lines $S_{1,0}$ divides the initial conditions into two segments, each promoting transport in different directions. For the segment lying to the left of $S_{1,0}$ the flow is in the direction of positive $q$, while in the segment to the right of $S_{1,0}$ the flow moves in the direction of negative $q$. Crucially, there is an imbalance in the size of the segments, and thus initially there is an unequal number of trajectories moving towards the two chaotic saddles located at the intersections of $S_{1,1}$ and $S_{1,-1}$ with $S_2$. This imbalance and the fact that the system contains an open component allows for the emergence of a non-zero directed current.

Previously, it has been stated that broken spatial-symmetries are of no consequence (with respect to the current) for systems with an energy surface entirely populated with initial conditions. However, the above discussion shows that for localised initial conditions broken symmetries play an important role. Namely, the asymmetric $V(Q)$ breaks time-reversibility for the localised initial conditions described above. Moreover, using a different potential $V(Q)$, which is invariant under reflections in $Q$, would restore the symmetry between counterpropagating trajectories, leading to a zero current.

To conclude this chapter, numerical results illustrating the cumulative effect of broken spatial symmetries and localised initial conditions on Model Two are presented. The effect that the anharmonic oscillator $V(Q)$ (asymmetric in $Q$) has varies as the coupling parameter $D$ is changed. To see this, the current as a function of $D$ is shown in Fig. 3.5. The explicit formula defining the current is given by Eq. (2.5). The simulation time is $T = 10^5$, with $N = 2 \times 10^5$ initial conditions (the construction of which is given above in this section).
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There exists a non-zero current in the range $0.48 \lesssim D \lesssim 1.18$ outside of which a zero current returns. It is clear, with the exception of a few $D$ values, that in this window of non-zero current the direction of the current is in the positive $q$ direction. The current reaches its largest value at $D \approx 0.75$. For all $D \neq 0$ time-reversibility symmetry has been broken, thus creating conditions conducive to a non-zero current. However, weak interactions for $D \lesssim 0.48$ means that an appropriate energy exchange between the washboard and deposit degrees of freedom does not take place. For interactions with $D \gtrsim 0.48$, the effects of the broken spatial symmetry become pivotal to the system dynamics. Indeed, it is because of the geometry of the anharmonic oscillator that, in the window $0.48 \lesssim D \lesssim 1.18$, the current is almost exclusively positive.

The return of zero net current at $D \approx 1.18$ seems to contradict much of the analysis in this chapter. However, even though the time-reversal symmetry has been broken through the use of the asymmetric $V(Q)$ and localised initial conditions, by Theorem 2.1, for $D \gtrsim 1.18$ there is insufficient system energy for the washboard particle to overcome the potential barriers $E_b$ and to undergo directed transport, thus precluding any possibility of a non-zero net current.
3.4 Chapter Summary

The breaking of the spatial and temporal symmetries are a prerequisite for the generation of a non-zero net current. Crucially, for the class of systems explored in Part I of this thesis time-reversibility symmetry is obeyed. Thus, for energy surfaces entirely populated with initial conditions (if achievable at all in practice) a non-zero net current is impossible. This is because each solution of the system is related to a corresponding solution such that they negate each others contribution to the net current. However, in this chapter it has been demonstrated that sets of localised initial conditions (which are frequently used for applications) can be enough to break this symmetry and allow for the occurrence of a non-zero net current. In the case of initial conditions that are unbiased with respect to the momentum, this may further require the breaking of spatial symmetry. Thus, the situation arises where the counterpart of an initial condition (that generates the counterpropagating trajectory) may not be contained in the set of initial conditions under consideration. In terms of current generation, an imbalance now exists.

It is worth re-emphasising that the mechanism responsible for the non-zero net current presented in this chapter is novel in that it doesn’t require a mixed phase-space, induced by time-periodic driving, consisting of regular and chaotic components (Flach et al., 2000; Yevtushenko et al., 2000). Rather, for the autonomous systems discussed here chaos is only needed in an initial stage of the dynamics to guide trajectories onto regular paths. After the finite period of transient chaos, the particles subsequently undergo regular rotational motion. This is in contrast to the sticking episodes close to tori, of finite duration, that provide a non-zero net current in the non-autonomous Hamiltonian case.

A step in this direction, i.e. of directed transport in autonomous systems, was taken by Dittrich & Naranjo (2010). In a three degree-of-freedom system, modelling a molecular motor, the external time periodic driving was replaced by an autonomous
degree-of-freedom that acts as an energy store. They observed that energy was able to propagate through the system resulting in directed transport. However, their results differ from the results presented in this chapter in two respects. Firstly, transport in the molecular motor model was aided by thermal fluctuations. Secondly, although on the one hand noise aided transport, on the other it also had the effect of destroying transport. Thus, the intervals transport (which are of finite duration) are separated by periods of bounded motion.

Much of this chapter has focused on the outcomes, related to transport, that can be observed when certain system symmetries are broken. Little attention has been given to the underlying structures in configuration space that facilitate these outcomes. By structures it is meant the equilibria and manifolds that guide the flow. The next chapter deals with these structures and how they are affected by broken symmetries. Particular attention will be given to exploring the differences in configuration space for the coupled and uncoupled systems.
CHAPTER 4

Manifolds and Saddles

The previous chapter examined the symmetry properties for the class of Hamiltonian systems given by Eq. (I.1), and the effect of broken symmetries for this class of systems. These effects were viewed primarily in terms of directed transport and current generation. Another important consequence of breaking (spatial) symmetries is to be found in configuration space where the location and properties of equilibria become distorted. In an abstract sense it is not easy to state what role this distortion will play in the overall system dynamics. However, it is clear that for the systems described previously, this distortion is of great importance with regard to the escape of trapped particles. To be precise, the interaction of the subsystems can cause the breaking of separatrices connecting neighbouring saddles and allow previously trapped particles to escape and subsequently undergo directed transport. By extension, the manifolds emanating from these equilibria also become distorted. Obtaining information about these manifolds is crucial as they organise the global dynamics. What happens to the unstable manifolds will be particularly important as transporting trajectories will follow these manifolds to escape from the interaction region.

This chapter will look firstly at systems when their degrees-of-freedom are uncoupled. The location of equilibria will be mapped out and their properties described. This is important as the main part of the chapter will explore how configuration space
changes in the coupled regime. For practical purposes, Model One and Model Two will be used as example systems.

4.1 Interaction Induced Changes in Configuration-Space

Consider a Hamiltonian system, with constant energy $E$, of the form Eq. (I.1) with $U(q)$ being the washboard potential and a second potential $V(Q) \geq 0$. These potentials are coupled via the interaction potential Eq. (I.4) with coupling parameter $D$. For the systems considered here this additional potential must have at least one minimum. For now, the case where there is more than one minimum will not be looked at in much detail as it is trivial matter to extend the description of configuration space to the case where the second potential has more than one minimum (this is looked at in § 4.2). Also, without loss of generality, it is reasonable to assume that the minimum of the additional potential is at the origin, i.e. $V(0) = 0$.

The properties of the washboard potential were discussed in the introduction to Part I. Of relevance here is that the washboard potential has minima located at $q_{\text{min}} = n$, with $U(q_{\text{min}}) = 0$, and maxima at $q_{\text{max}} = n + 0.5$, with $U(q_{\text{max}}) = 1/\pi \, (\approx 0.318)$, where $n \in \mathbb{Z}$.

Let us first consider the case when the potentials are uncoupled ($D = 0$). Thus for the combined system with potentials $U(q)$ and $V(Q)$ the configuration space $(q, Q)$ contains equilibria located at various points located along the line $Q = 0$. These equilibria are of two types, namely centre-centre and saddle-centre. The centre-centre equilibria are formed where the minima of the potentials $U(q)$ and $V(Q)$ meet. While the saddle-centre equilibria are formed when the minima of the potential $V(Q)$ meets a maximum of $U(q)$. To be precise the centre-centre equilibria are located at
4.1. CHANGES IN CONFIGURATION-SPACE

the points \((n, 0)\), and the saddle-centre equilibria are located at \((n + 0.5, 0)\) where \(n \in \mathbb{Z}\). Importantly, as there is no interaction between the potentials the height of the potential barriers, along the \(q\)-coordinate, retains the energetic height defined by the washboard potential. That is, the saddle-centre equilibria each have a height of \(1/\pi\).

The dynamics in configuration space for the uncoupled potentials is relatively uneventful as the system is integrable and no complex dynamics can exist. Depending on the system’s energy there are a number of possible outcomes. Firstly, as the subsystems do not interact and exchange energy they can be considered separately. For the washboard potential two situations can arise: the energy \(E_w\) contained in the washboard particle is less than the washboard barrier height — \(E_w \leq 1/\pi\), or it is greater than the barrier height — \(E_w > 1/\pi\). If the former is true, then the particle will be unable to overcome the washboard barriers and will be trapped in one of its potential wells undergoing librational motion. If the latter is true, then the particle will be able to overcome all of the washboard barriers and will thus undergo rotational motion escaping to infinity. Turning to the second potential \(V(Q)\) only one situation arises. That is, the particle will oscillate about the potential minimum, with the size of the oscillations depending on the subsystem’s energy.

The location and properties of the equilibria change as the system enters the coupled regime \((D \neq 0)\), and consequently the dynamics become more complex. The changes in the equilibria are two-fold. The locations of the equilibria are altered due to the energy exchange between the subsystems. This change is clearly evident when \(|q - Q| \approx 0\) and the energy exchange is most prominent. In the range \(|q - Q| \to \infty\) the particles effectively decouple and the equilibria locations maintain their positions from the uncoupled regime. The second change is related to the height of the equilibria and this has important consequences for particle transport. Recall that \(H_{\text{int}}(q, Q) \to D\) as \(|q - Q| \to \infty\). The implication for the equilibria is that in the asymptotic range their potential height increases by \(D\) units. To approach this from a different point of
view, as the two particles move apart they sacrifice energy to the interaction potential. Contrasted with this is the uncoupled case where the two subsystems maintain their respective energies regardless of the positions they have in the potential landscape.

The splitting of the invariant manifolds induced by the interaction potential creates a non-attracting chaotic set called a chaotic saddle. There appear notable consequences of these chaotic saddles which include chaotic scattering and transient chaos (Ott, 1992; Ott & Tél, 1993). The transient dynamics enhance the possibility of a cooperative escape of the washboard particle. The effect of this desymmetrisation of the equilibria, and by extension the effect of the chaotic saddles, on the different transport scenarios is best illustrated by example. For this we return to Model One and Model Two.

4.2 Desymmetrisation of Saddles

Let us recall the set-up of Model One. There are two washboard potentials, coupled via the interaction potential $H_{\text{int}}$. The initial conditions are chosen such that one particle is at rest at the origin, while the other is outside the interaction region with momentum bringing it in the direction of the particle at rest (for a more thorough description of the system and the initial conditions see § 2.1). As Fig. 2.5 has shown, the dynamics of the system are sensitively dependent on the strength of the coupling. For a low $D$ value, particle $A$ can pass through the interaction region unscathed. With increasing $D$, particle $A$ can no longer find a direct route through the interaction region. Instead, it enters into an energy exchange with particle $B$ with both particles trying to find a path out of the interaction region. As previously discussed, there are numerous possible scenarios for particles $A$ and $B$, once particle $A$ has reached the interaction region. In short, these scenarios are characterised by the duration of the chaotic motion, ranging from zero duration (no chaos) in the
uncoupled case, through transient periods of chaos, to infinity (persistent chaos) in the strongly coupled case. It should be said that the duration of chaotic motion for a trajectory is also sensitive to changes in its initial condition. A partial explanation for these above mentioned scenarios, and indeed the duration of chaotic motion, comes from the saddle point energies corresponding to the various $D$ values.

In Fig. 4.1, some of the locations of the equilibria of the system (for $D = 0.58169$), in the range $-10 \leq q \leq 10$ and $-0.7 \leq Q \leq 0.7$ are shown in the $(q, Q)$-plane *. Let $(q_i, Q_j)$ denote the equilibrium point. In the uncoupled case $q_i \simeq i/2$ and $Q_j \simeq j/2$, i.e. these are the equilibria of the corresponding washboard potentials. In addition to the two types of equilibria described in the previous paragraphs, Model One also possesses a third type of equilibria – the saddle-saddle equilibria. This third type of equilibria results when both potentials $U \& V$ each have maxima. The saddle-saddle equilibria are located at the intersection of these maxima. In more detail, when the Hamiltonian system is linearised about an equilibria, it will produce two pairs of eigenvalues. The equilibria is said to be of saddle-saddle type if the eigenvalues take the form $\pm \lambda_1, \pm \lambda_2$ where $\lambda_{1,2} > 0$. It is said to be of saddle-center type if the eigenvalues take the form $\pm \lambda_1, \pm i\lambda_2$ where $\lambda_{1,2} > 0$ and $i$ is used to indicate an imaginary number.

The distortion in configuration space, when the particles are coupled, is clear to see. Notably, there is a lack of $q \mapsto -q$ and $Q \mapsto -Q$ reflection symmetry. It is this distortion which allows particle $B$ (for the considered initial conditions) to become excited and potentially leave its starting potential well. The reason being that, with the path of least resistance no longer being along the line $Q = 0$, particle $A$ deviates from its hitherto straight line path and thus stimulates particle $B$.

Fig. 4.2 shows saddle point energies as a function of $D$. The left panel, corresponding to the saddle points $(0, 2i + 1)$, indicates that all of these saddle points are

*The locations of the equilibria in this figure (and those to follow) have been found numerically, to a high degree of accuracy, using Newton’s method.
energetically accessible for every $D < D_{\text{crit}} \approx 0.5817$ (cf. Theorem 2.1) when the system’s energy is $E = 0.9$ (which is used in all numerical simulations for Model One). In fact, while $D < D_{\text{crit}}$ this holds true for all $i \rightarrow \pm \infty$ as the saddle energies increase by $D$ units in this asymptotic limit, approaching $D + 1/\pi$ from below – which is the system’s energy. In contrast, many of the saddle points $(1, 2i + 1)$ (right panel) become energetically inaccessible after a relatively small $D$ value ($D \approx 0.3$). This suggests that these inaccessible saddles form the boundaries of channels guiding the particles. Crucially, even though the paths may be blocked at many points, there are still multiple routes for the particles to wander and thus the possibility of a directed current being produced is not excluded. In this sense, the inaccessible saddles are a source of particle scattering as approaching particles deflect away from these saddles seeking out energetically accessible regions of phase-space. This is analogous to the scattering problem studied by Tél et al. (1993), where particles evolve in a potential that consists of multiple ‘hills’, in which chaotic scattering results when the system’s energy falls in a range that is lower than the maximum potential energy.
Another interesting observation that can be made from these figures is that above $D \approx 0.12$ the saddle energies create barriers that, with the simulation energy $E = 0.9$, only one particle can pass over. In particular, some of the saddle energies attain values greater than 0.45 which eliminates the possibility of both particles undergoing independent escapes (cf. § 2.3). Below $D \approx 0.12$, it is energetically feasible that both particles can have enough energy to mount independent escapes. However, the low coupling strength excludes the possibility of particle $B$ attaining enough energy from the interaction with particle $A$. Therefore in general, if one particle escapes, it will be at the expense of the other which must remain trapped for the entire simulation.

The green lines (negative slope) superimposed on both plots in Fig. 4.2 going from the points $(0.0, 0.9)$ to $(0.5817, 1/\pi)$ show the initial energy of particle $A$ as a function of $D$. In the left plot we see that for $D \lesssim 0.28$ particle $A$ will initially possess enough energy to overcome all of these barriers. Increasing $D$ beyond this value will mean that the scattering nature of this system will become more pronounced. Rather than going over these potential barriers, particle $A$ must now find alternative routes around them. This means that a significant interaction will ensue and that particle $B$’s role in the dynamics will be fundamental. A similar situation unfolds in the right hand plot. However, many of the saddle points become energetically inaccessible for increasing $D$, meaning that the particles will be unable to obtain enough energy from the interaction potential to overcome these barriers.

The scenario with a vanishingly small current (i.e. $D = 0.58169$) still requires an explanation. Examining the saddle point energies at this $D$ value (shown by a vertical line in the plots) we see that almost all of the saddle points $(1, 2i+1)$ are energetically inaccessible. Only those saddle points $(1, 1)$ and $(1, 3)$ can be overcome. As already noted, all of the saddle points $(0, 2i+1)$ are energetically accessible. However, those saddle points with $i > 4$ have energies that tend to 0.9. Thus for a particle to pass over these barriers requires that the particle holds all energy contained in the system. The strength of the coupling almost certainly precludes such a situation and therefore
both particles are forced to wander chaotically in the interaction region. Importantly, as $D$ increases, so does the size of the energetically inaccessible regions. With increasing $D$, these regions join forming an impenetrable barrier that the particles cannot pass, and thus leaving them to wander in the interaction region. This is depicted in Fig. 4.3.

### 4.3 Manifolds

Turning to Model Two where the additional potential is asymmetric in its coordinate it can be seen in Fig. 4.4 (for $D = 0.75$) that the inclusion of the interaction
potential has a similar effect on the location of the system’s equilibria as can be seen in Model One. That is, there is a distortion in the interaction region. For the discussion concerning the saddles of Model Two, the concise notation $x_i = (q_i, Q_i)$ will be used, as the additional potential $V(Q)$ contains only a single equilibria. Where Model One and Model Two differ is that the respective additional potentials shape the nature of the equilibria in different ways. Crucially, unlike in Model One, the centre-saddle and centre-centre equilibria from Model Two confine any possible transport to one direction in coordinate-space. Further, just like in Model One, the interaction potential causes an increase in the equilibrium point energies. The increase in energy depends on the coupling strength $D$, where the energies monotonically grow with increasing $D$.

To see how a transporting trajectory manipulates its way through the asymmetric potential landscape, the example trajectory shown in Fig. 3.1(b) is projected onto coordinate-space and onto the effective potential (see Fig. 4.5). During an initial chaotic transient with both particles in the interaction region, an energy redistribu-
4.3. MANIFOLDS

Figure 4.4: Locations \((q_i, Q_i)\) of the \(i\)-th equilibrium point \(x_i\) in configuration space, for \(-20 \leq i \leq 20\), for \(D = 0.75\). Centre-centre equilibria are indicated by circles (green); saddle-centre equilibria are indicated by crosses (red).

The effect of the asymmetry on the dynamics of the system in the interaction region takes place with the energy deposit, i.e. the anharmonic oscillator. Subsequently, the washboard particle manages to escape from the interaction region and thereafter exhibits sustained directed motion of rotational type. Notably, the anharmonic oscillator retains some energy which causes librational motion in the \(Q\)-coordinate. The asymmetry in the interaction region of the effective potential is also clear from this figure. However, asymptotically as \(q \to \infty\) the \(q \to -q\) symmetry of the washboard potential is restored as the two degrees-of-freedom effectively decouple leaving two almost integrable subsystems.

The asymmetry is reflected in the energies of the equilibria only in a subtle manner; Fig. 4.6(a) shows the energies at the equilibria, while Fig. 4.6(b) illustrates the energetic barrier heights (between successive saddles and centres). While the difference in energy between successive barriers is small, it can play an important role in the overall system dynamics, as will be seen below when the manifolds emanating from the equilibria are considered.
Figure 4.5: An escaping trajectory, for coupling strength $D = 0.75$, shown with the effective potential surface and equipotential curves. The total energy is $E = 1.5$.

gion is illustrated by the stable/unstable manifolds of the saddles $x_{-1}$ and $x_1$, shown in Fig. 4.7. It seems that the stable/unstable manifolds branches of both equilibria, that move toward the origin, get caught in a bottleneck in the energy surface. However, the manifold branches emanating from the equilibria $x_{-1}$ (with $\dot{q} > 0$) eventually passes through the bottleneck and subsequently negotiates its way past the saddle $x_1$ and into the neighbouring potential well. In contrast, the manifolds branches emanating from $x_1$ (with $\dot{q} < 0$) are unable to pass the saddle $x_{-1}$.

Due to the bounded nature of the anharmonic potential, in the asymptotic limit $|q| \to \infty$, the interaction vanishes and only the influence of the washboard remains.
The saddles in this system are then connected by a chain of heteroclinic connections stretching in both the positive and negative $q$ direction. This results in a symmetry-like situation in that the dynamics taking place in a window containing the region $q_{2k+1} \leq q \leq q_{2k+2}$ matches that in the region $q_{2(k+1)+1} \leq q \leq q_{2(k+1)+2}$. Indeed, as long as the particles remain sufficiently far apart, this is true for all $k$.

However, for finite $|q|$, the interaction term, however small, introduces a local asymmetry in the energy surface about each saddle point. Specifically, the saddle point energies $U_{\text{eff}}(x_{\pm(2k+1)})$ ($k > 0$) are monotonically increasing as one moves away...
4.3. MANIFOLDS

Figure 4.7: Stable/unstable manifold branches of the saddle points $x_{-1}$ with $q_{-1} \simeq -0.5$ (a) and $x_{+1}$ with $q_{+1} \simeq 0.5$ (b).

from the origin (increasing $k$). The heteroclinic connections of the washboard system are no longer permitted on energetic grounds. Stable and unstable manifold branches of saddle points $x_{\pm(2k+1)}$ ($k > 0$) whose initial segments point away from the origin are confined to the neighbouring potential wells associated with the equilibria $x_{\pm(2k+2)}$ since the associated energy surface does not extend as far as the saddles at $x_{\pm(2k+3)}$.

This ‘local’ asymmetry about each saddle point occurs in the same manner for both negative and positive $q$. However, following the ‘inward-facing’ stable/unstable manifold branches of saddle points, i.e., those with initial segments oriented towards the origin ($\dot{q} > 0$ for $q < 0$ and $\dot{q} < 0$ for $q > 0$) that enter the region of strongest
interaction with the energy deposit, reveals a significant asymmetry in the long-range
dynamics, illustrated by computing the stable/unstable manifold branches of the
saddles at $x_{-19}$ and $x_{+19}$, shown in Fig. 4.8.

Energetic constraints mean that the stable/unstable manifold branches of the
saddle at $x_{-19}$ with $\dot{q} < 0$ (i.e., the left-hand branches) are confined to the well
associated with $x_{-20}$; they cannot extend beyond the saddle at $x_{-21}$. Similarly, the
stable/unstable manifold branches of the saddle at $x_{+19}$ with $\dot{q} > 0$ (i.e., the right-
hand branches) are confined to the well associated with $x_{+20}$; they cannot extend

Figure 4.8: Stable/unstable manifold branches of the saddle points
$x_{-19}$, with $q_{-19} \simeq -9.5$, and $x_{+19}$, with $q_{+19} \simeq +9.5$. Here, $D = 0.75$.
The line $q = 0$ is shown (dashed).
beyond the saddle at $x_{+21}$.

The branches for $x_{\pm 19}$ appear, at first, to be symmetric partners; both remain close to the $Q$-axis, the system having almost all of its energy in the washboard degree-of-freedom. However, their behaviours after entering the interaction region differ significantly: the branch emanating from $x_{+19}$ passes as far as the well associated with $x_{-4}$ by which time redistribution of energy between modes associated with the washboard and the deposit mean that it has insufficient energy in the washboard mode to pass the saddle at $x_{-5}$. After further passage through the interaction region, it enters the well associated with $x_{-8}$ but is again deflected in the neighbourhood of the saddle at $x_{-9}$. Although the trajectory has sufficient total energy to overcome the energetic barrier between the wells associated with $x_{-8}$ and $x_{-10}$ at this point, the energy is no longer distributed suitably between the available modes of the system. After a number of passes through the interaction region, the branch reaches a turning point and retraces its steps out of the interaction region. Markedly different behaviour is observed for the branch emanating from $x_{-19}$: an initial segment of this branch, followed by integrating numerically an initial condition over the same time period as the branch described above, does not extend beyond the saddle at $x_{+5}$, instead crossing and re-crossing the centre of the interaction region repeatedly over the integration time. In conclusion, we have demonstrated that the local interaction with the anharmonic oscillator produces a significant desymmetrisation of the saddles and their associated stable/unstable manifolds (and hence the long-range dynamics). This has important consequences for transport, and the net current, as ultimately these saddles collectively determine the direction of the particle flow.
4.4 Chapter Summary

To thoroughly understand the dynamics of a system it is crucial to have knowledge of the system’s equilibria and, more importantly, the manifolds emanating from the unstable equilibria, as it is these structures that organise the system’s dynamics on a global scale. This chapter has explored these structures for the class of Hamiltonian systems given by Eq. (I.1) and paid particular attention to how these structures are distorted by the coupling potential.

In the uncoupled case the saddles form a symmetric chain of points, along the washboard degree-of-freedom, with heteroclinic connections connecting neighbouring saddles. Moreover, this symmetry property holds true for all equilibria; that is, along the washboard degree-of-freedom, the system is symmetric about every equilibria point.

This situation changes drastically when the coupling strength becomes non-zero. With regard to the saddles, there is a change in position in coordinate-space. This change is most pronounced in the interaction region, i.e. where $q \approx Q$. However, in the asymptotic limit, the two subsystems effectively decouple and the position of the equilibria is restored. Further, there is an increase in the potential energy associated with each equilibria. This increase is related to the location of the equilibria and the coupling strength $D$. Moving away from the origin, along the washboard degree-of-freedom in both the positive and negative directions, sees the saddle energies increase. Also, the saddle (centre) energies increase monotonically with increasing distance from the origin. In the asymptotic limit $q \to \pm \infty$ the potential energies of the equilibria increase by $D$ units with respect to their uncoupled counterpart.

The stable/unstable manifold branches emanating from the system’s saddle points are also subject to the asymmetry induced by the coupling potential. First of all, as the saddle energies are monotonically increasing (with distance from the origin), each saddle point has a local asymmetry associated with it. In addition, for some saddle
point located at \((q_s, Q_s)\) (outside the interaction region) and its counterpart located at approximately \((-q_s, Q_s)\), the subtle difference in energy of these saddles means that the dynamics preceding to the left and to the right can be extremely different.

It is important to note that these changes to the system’s saddles and corresponding manifolds are the product of an asymmetry induced by the coupling potential. This is true in that symmetry is restored for vanishing coupling strength, along the washboard degree-of-freedom, regardless of the type of additional potential \(V(Q)\) used, which can be asymmetric or otherwise.
Part II

Transport in Non-autonomous Systems
Introduction

In Part I the Hamiltonian dynamics of autonomous systems of two coupled oscillators were explored. This part will continue in a similar vein. However, the equations of motion will be augmented by the inclusion of driving and damping terms adding further complexity to the coupled dynamics. Further, the short range interaction potential Eq. (I.4) (which allows for the occurrence of certain phenomena, in particular transient chaos) will be replaced by a potential that allows for long range interactions between the particles.

Again, the systems will consist of two coupled particles each evolving in a washboard potential. The particles are driven by a time periodic force and damped. These systems are nonautonomous and without conservation of energy. They have equations of motion

\[ \ddot{q}_1 = -\sin(2\pi q_1) - \gamma \dot{q}_1 + h_1 \sin(\Omega t + \theta_0) - \kappa(q_1 - q_2) , \]  
\[ \ddot{q}_2 = -\sin(2\pi q_2) - \gamma \dot{q}_2 + h_2 \sin(\Omega t + \theta_0) + \kappa(q_1 - q_2) , \]

where \( \gamma \) is the strength of the damping, \( h_{1,2} \) are the driving amplitudes, and \( \Omega, \theta_0 \) are the driving frequency and phase respectively. \( \kappa \) represents the strength of the linear coupling between the two particles. For the remaining chapters the variables \( q_1, q_2, p_1, p_2 \) will be used, rather than the notation \( q, Q, p, P \) used in Part I.

The focus of Part II is on how the coupling strength influences the dynamics of the system above (Eq. (II.1) and Eq. (II.2)). However, it is useful for what is to come to understand the uncoupled dynamics (\( \kappa = 0 \)) of this system (Hennig et al., 2009b). That is, the dynamics of a single driven and damped particle evolving in a washboard potential. The dissipative nature of this system means that all orbits will eventually evolve to one of the systems, possibly coexisting, attractors. The type of attractors present will depend on the parameters used, while the particular attractor
that an orbit evolves to is dependent on the initial condition. This is illustrated in Fig. II.1 where two qualitatively different attractors are shown. The parameters used are $\gamma = 0.1$, $\Omega = 2.25$, $\theta_0 = 0$. The strange chaotic attractor (blue) results when the driving amplitude is $h = 1.3$. Increasing this driving amplitude to $h = 1.5$ results in the periodic attractor (red). With regard to a net current the transporting orbits evolving on the periodic attractor will yield a non-zero net current, whereas the trajectories landing on the strange chaotic attractor are, on long time scales, typically expected to produce a vanishingly small contribution to the net current. However, as will be seen later, it is possible for trajectories evolving on a chaotic attractor in a higher dimensional phase-space to produce a non-zero current.

![Figure II.1:](image)

Figure II.1: Left panel: Stroboscopic map with sampling frequency $2\pi/\Omega$. Shown are the strange (blue) and periodic (red) attractors corresponding to driving strengths $h_1 = 1.3$ and $h_2 = 1.5$ respectively, in the uncoupled regime. The remaining system parameters are $\gamma = 0.1$, $\Omega = 2.25$, $\theta_0 = 0$, and $\kappa = 0.0$. The coordinates $q$ are given $\mod (1)$. The dot (red) has been enlarged for emphasis. Right panel: A corresponding example trajectory for motion on the strange (blue line) and periodic (red line) attractor.

Thus, the single particle system is a rich source of interesting dynamics. The
full system, Eq. (II.1) and Eq. (II.2), presents a further opportunity for new and interesting behaviours. For now consider the uncoupled case $\kappa = 0$. Thus, depending on the strength of the driving amplitudes $h_1$ and $h_2$ (with the remaining parameters as given above), there are a number of possible combinations of attractor for the underlying subsystems. For driving amplitudes $h = 1.3$ (strange chaotic attractor) and $h = 1.5$ (regular attractor) there are three combinations of attractors for the underlying subsystems - regular/regular, regular/strange, and strange/strange. The complexity of this system arises when the two subsystems are coupled, i.e $\kappa \neq 0$.

With a view to the discussion in Chapter 3 regarding symmetries, it is worth briefly exploring the symmetry properties of this system which now includes driving and damping terms. To begin, let us assume equal driving amplitudes $h_1 = h_2$. Firstly note that the particle exchange symmetry $q_1 \rightarrow q_2, q_2 \rightarrow q_1$ is preserved. Thus synchronous solutions, for example, are permitted. However, time-reversibility is broken here due to damping, meaning that these systems have a clear direction of time (which is easily verified by applying the time-reversal operator to the equations of motion). This is a generic feature of dissipative systems. The implication is that applying the time-reversal operator to a forward trajectory does not necessarily produce another trajectory that is permitted under the equations of motion. Going further, the corresponding backward trajectory that would cancel the forward trajectories contribution to the net current is not obtained through the time-reversal operation. In this sense, all sets of initial condition will be biased. This is only a necessary condition for the generation of a non-zero net current. The actual current will be determined by the basins of attraction in which the initial conditions lie, and by extension their corresponding attractors. Finally, in the case of unequal driving amplitudes $h_1 \neq h_2$ the above discussion on time-reversibility is still valid. The difference now is that the particle exchange symmetry is broken, and thus synchronous motion becomes hindered (except in the range of very strong coupling between the units).
Part II is organised as follows. This part begins in Chapter 5 with a perturbational analysis of the system described by Eq. (II.1) & Eq. (II.2). In particular, Melnikov’s homoclinic method is employed to determine when the onset of chaos will occur as a function of the system’s parameters. In addition, this chapter will look at the transport features present in the system. Chapter 6 is dedicated to the study of three example model systems. These models each have interesting and contrasting dynamics. They are described by the underlying attractors of the subsystems as, in order, strange vs strange attractors, strange vs regular attractors, and regular vs regular attractors respectively.
CHAPTER 5

Analytical Results

Chaotic solutions of a system quite often contribute nothing when it comes to the emergence of a net current. It is therefore important to understand the nature and prevalence of chaos in a system. Further, it useful to know the conditions under which a system can exhibit chaotic solutions.

One of the few analytical methods for determining the existence of chaotic solutions in a system is due to Melnikov. In brief, this method relies on the unperturbed homoclinic orbit emanating from a hyperbolic fixed point to test for transversal intersections of its stable and unstable manifolds when the integrable system has been perturbed. In this situation theorems due to Moser and Smale can be applied to conclude that such a system is chaotic (Wiggins, 1990).

Melnikov’s method is particularly useful in the study of dissipative systems. The reason being that the perturbed stable/unstable manifolds do not necessarily intersect transversally in dissipative systems.
5.1 Melnikov Analysis

Of particular interest is the influence of the coupling between the particles to the overall system dynamics. In this section, using Melnikov’s method, information will be extracted from the system that will illuminate the complicated dependence of the dynamics on the coupling strength. In particular, information of a homoclinic bifurcation, suggesting the onset of chaos, will be derived.

Before proceeding, the system of equations Eq. (II.1)-(II.2) is reformulated so that it is in a form suitable for a perturbative analysis. For weak driving, damping, and coupling the equations become

\[
\begin{align*}
\ddot{q}_1 + \sin(2\pi q_1) &= \epsilon \left( -\gamma \dot{q}_1 + h_1 \sin(\Omega t + \theta_0) - \kappa(q_1 - q_2) \right), \\
\ddot{q}_2 + \sin(2\pi q_2) &= \epsilon \left( -\gamma \dot{q}_2 + h_2 \sin(\Omega t + \theta_0) + \kappa(q_1 - q_2) \right),
\end{align*}
\]

where \(0 < \epsilon \ll 1\) in the perturbative regime. Setting \(\epsilon = 0\) these equations reduce to two unperturbed (uncoupled) simple pendula, both being integrable. That is

\[
\begin{align*}
\dot{p}_i &= -\sin(2\pi q_i), \\
\dot{q}_i &= p_i, \\
i &= 1, 2.
\end{align*}
\]

There exist hyperbolic fixed points given by

\[
(\bar{p}_i, \bar{q}_i) = \left( 0, \pm \frac{1}{2} \right),
\]

Let us consider for a moment a single unperturbed pendulum. This has an elliptic fixed point at \((0, 0)\) – corresponding to the pendulum facing vertically downwards – and hyperbolic fixed points at \((0, \pm 1/2)\) – corresponding to the pendulum facing vertically upwards. Of interest here are the hyperbolic fixed points, as a heteroclinic connection exists between these fixed points. Crucially, the stable and unstable manifolds making up this heteroclinic connection coincide in phase-space, implying that the motion of the pendulum is regular.
Returning to the full unperturbed system, consisting of the two pendula, in the $p_1 - q_1 - p_2 - q_2 - \theta$ space the system has a hyperbolic periodic orbit

$$
\mathcal{M} = (p_1, q_1, p_2, q_2, \theta(t)) = \left(0, \pm \frac{1}{2}, 0, \pm \frac{1}{2}, \Omega t + \theta_0\right).
$$

This hyperbolic periodic orbit is connected to itself by two pairs of homoclinic trajectories given by (see Appendix A for derivation)

$$
(p_{1h}^\pm(t), q_{1h}^\pm(t), p_{2h}^\pm(t), q_{2h}^\pm(t), \theta(t)) = \left(\pm\sqrt{\frac{2}{\pi}} \ \text{sech} \left(\sqrt{2\pi} t\right), \pm \frac{1}{\pi} \ \text{sin}^{-1} \left[\text{tanh} \left(\sqrt{2\pi} t\right)\right], \pm\sqrt{\frac{2}{\pi}} \ \text{sech} \left(\sqrt{2\pi} t\right),
$$

$$
\pm \frac{1}{\pi} \ \text{sin}^{-1} \left[\text{tanh} \left(\sqrt{2\pi} t\right)\right], \Omega t + \theta_0\right). \quad (5.6)
$$

$\mathcal{M}$ has three-dimensional stable and unstable manifolds which coincide along four three-dimensional sets of homoclinic orbits, denoted by $\Gamma^\pm$, which can be parametrised as

$$
\Gamma^\pm = \left\{ (p_{1h}^\pm(-\tau_1), q_{1h}^\pm(-\tau_1), p_{2h}^\pm(-\tau_2), q_{2h}^\pm(-\tau_2), \theta_0) \right. \left| (\tau_1, \tau_2, \theta_0) \in \mathbb{R}^1 \times \mathbb{R}^1 \times T^1 \right\}. \quad (5.7)
$$

The real parameters $\tau_{1,2}$ determine the position on the homoclinic orbits. To determine whether the stable and unstable manifolds intersect transversely we compute the Melnikov integrals (for details concerning the Melnikov method in higher dimensions see Wiggins (1988); Yagasaki (1999a,b))

$$
M_i^{\pm}(\tau_1, \tau_2) = \int_{-\infty}^{\infty} \left\{ p_{ih}^\pm(t - \tau_i) \left[-\gamma p_{ih}^\pm(t - \tau_i) - h_i \sin(\Omega t + \theta_0) \right]
$$

$$
+ \kappa \left( q_{i+1h}^\pm(t - \tau_{i+1}) - q_{ih}^\pm(t - \tau_i) \right) \right\} dt. \quad (5.8)
$$
The integration is performed over the homoclinic trajectories given in Eqs. (5.6) yielding the following integrals

\[ I_\tau = \int_{-\infty}^{\infty} \left\{ \pm \sqrt{\frac{2}{\pi}} \tanh \left( \sqrt{\frac{2}{\pi}} \left( t - \tau_i \right) \right) \right\} \left[ \mp \sqrt{\frac{2}{\pi}} \tanh \left( \sqrt{\frac{2}{\pi}} \left( t - \tau_i \right) \right) \right] \ \text{for} \ i = 1, 2, \ \tau_3 = \tau_1, \ \& \ q_{3h}^\pm = q_{1h}^\pm. \]

Using the method of residues we obtain for the case of equal signs

\[ M_1^{(\pm, \pm)}(\tau_1, \tau_2) = -2\gamma \sqrt{\frac{2}{\pi^3}} \mp h_1 \text{sech} \left( \sqrt{\frac{\pi}{2}} \frac{\Omega}{2} \right) \sin(\Omega \tau_1) + \frac{\kappa}{\pi^2} I(\Delta \tau), \]

and

\[ M_2^{(\pm, \pm)}(\tau_1, \tau_2) = -2\gamma \sqrt{\frac{2}{\pi^3}} \pm h_2 \text{sech} \left( \sqrt{\frac{\pi}{2}} \frac{\Omega}{2} \right) \sin(\Omega \tau_2) - \frac{\kappa}{\pi^2} I(\Delta \tau). \]

For unequal signs we obtain

\[ M_1^{(\pm, \mp)}(\tau_1, \tau_2) = -2\gamma \sqrt{\frac{2}{\pi^3}} \mp h_1 \text{sech} \left( \sqrt{\frac{\pi}{2}} \frac{\Omega}{2} \right) \sin(\Omega \tau_1) - \frac{\kappa}{\pi^2} I(\Delta \tau), \]

and

\[ M_2^{(\pm, \mp)}(\tau_1, \tau_2) = -2\gamma \sqrt{\frac{2}{\pi^3}} \pm h_2 \text{sech} \left( \sqrt{\frac{\pi}{2}} \frac{\Omega}{2} \right) \sin(\Omega \tau_2) + \frac{\kappa}{\pi^2} I(\Delta \tau). \]

The function \( I(\Delta \tau) \) is determined by the integral

\[ I(\Delta \tau) = \int_{-\infty}^{\infty} \frac{\sin^{-1} [\tanh(t + \Delta \tau)]}{\cosh(t)} \ dt, \]

(5.14)
where

\[ \Delta \tau = \sqrt{2\pi}(\tau_1 - \tau_2). \] (5.15)

Denoting \( t = \Delta \tau \), the function \( I(t) \) has the following properties

\[ I(0) = 0, \ I(t) = -I(-t), \ \frac{dI(t)}{dt} > 0, \ \text{and} \ \max_{t \in \mathbb{R}} |I(t)| = \lim_{t \to \pm \infty} |I(t)| = \frac{\pi}{2}. \] (5.16)

Without loss of generality assume that \( h_1 > h_2 \). From equations (5.10)-(5.13) it can be readily seen that if

\[ h_2 > \left(2\gamma\sqrt{\frac{2}{\pi^3}} + \frac{\kappa}{\pi^2}I(t)\right) \cosh\left(\sqrt{\frac{\pi}{2}}\Omega^{\pm}\right), \] (5.17)

then there are roots \( \tau_1, \tau_2 \in \mathbb{R} \) to the transcendental equations (5.10)-(5.13). Therefore, the Melnikov functions \( M^{(\pm, \pm)} \) and \( M^{(\pm, \mp)} \) have zeros. Furthermore, with

\[ \frac{\partial M_1^{(\pm, \pm)}}{\partial \tau_1} = \mp \tilde{F} \cos(\Omega \tau_1) + \tilde{I}, \quad \frac{\partial M_1^{(\pm, \pm)}}{\partial \tau_2} = -\tilde{I}, \] (5.18)

\[ \frac{\partial M_2^{(\pm, \pm)}}{\partial \tau_1} = -\tilde{I}, \quad \frac{\partial M_2^{(\pm, \pm)}}{\partial \tau_2} = \pm \tilde{F} \cos(\Omega \tau_2) - \tilde{I}, \] (5.19)

one obtains

\[ \det DM^{(\pm, \pm)}(\tau_1, \tau_2) = \pm [\cos(\Omega \tau_1) + \cos(\Omega \tau_2)] \tilde{F} - \tilde{F}^2 \cos(\Omega \tau_1) \cos(\Omega \tau_2) - 2\tilde{I}^2, \] (5.20)

with

\[ \tilde{F} = \Omega \sech\left(\sqrt{\frac{\pi}{2}}\Omega^{\pm}\right), \ \text{and} \ \tilde{I} = \frac{\kappa}{\pi^2} \frac{dI(t)}{dt}. \] (5.21)
Providing that \( \det DM^{(±,±)}(\tau) \neq 0 \) (\( \det DM^{(±,±)}(\tau) \neq 0 \)) then the homoclinic Melnikov vector \( M^{(±,±)}(M^{±}) \) has simple zeros implying transversal intersections of the stable and unstable manifolds (Wiggins, 1988; Yagasaki, 1999a,b).

Thus the conditions for the transverse intersections of the stable and unstable manifolds have been derived. From Eq. (5.17) and the properties contained in Eq. (5.16) it is possible to impose further constraints on the system’s parameters. Crucially, these properties impose a constraint on the magnitude of the product \( \kappa \cdot I(t) \) allowing one to obtain the following homoclinic bifurcation threshold

\[
h_c = \left( 2\gamma \sqrt{\frac{2}{\pi^3}} + \frac{\kappa}{2\pi} \right) \cosh \left( \sqrt{\frac{\pi}{2}} \Omega \right). \tag{5.22}
\]

For \( h_2 > h_c \) the existence of roots to the transcendental equations (5.10)-(5.13) is guaranteed giving birth to homoclinic orbits being of importance for the existence of strange attractors. Note that this bifurcation condition limits the maximal value of the coupling strength \( \kappa \) but is independent of the value of \( \Delta \tau \).

With further regard to the influence of the coupling strength \( \kappa \) on the behaviour of the stable and unstable manifolds the condition for the existence of zeros of the Melnikov functions, as given in (5.17), confines the magnitude of the product \( \kappa \cdot I(\Delta \tau) \), viz. relates the value of \( \kappa \) and \( \Delta \tau \). In fact, taking into account the properties of \( I(\Delta \tau) \) (see Eq. (5.16)) one concludes that the larger the coupling strength \( \kappa \) the smaller \( \Delta \tau \) has to be in order that the value of \( I(\Delta \tau) \) complies with the condition (5.17). That is, with increasing values of \( \kappa \) the points where the stable and unstable manifolds intersect each other transversely on the homoclinic orbits get closer to each other, giving evidence for the tendency towards synchronisation between the two particle oscillators. Eventually for \( \tau_1 = \tau_2 \) the ensuing ‘freezing of the dimensionality’ reduces the system to a single driven and damped pendulum (one-and-a-half degree of freedom system) which impedes the occurrence of hyperchaos as this is necessarily connected with expansions in several directions in phase space simultaneously (several
positive Lyapunov exponents). Nevertheless, for sufficiently small $\kappa$, simple zeros of the Melnikov functions with $\tau_1 \neq \tau_2$ exist allowing for the occurrence of hyperchaos.

### 5.2 Features of Transport

Departing from the perturbative approach of § 5.1, this section will examine a very particular type of solution for the full system. This solution, which will be named the *periodic running solution*, is desirable for achieving directed particle transport. The properties and consequences of such a solution will be dealt with in this section.

The periodic running solutions are characterised by

\[ q_i(t + T) = q_i(t) + m_i, \quad \dot{q}_i(t + T) = \dot{q}_i(t), \quad i = 1, 2, \quad (5.23) \]

where $T$ is the duration of the period, and the $m_i$ are constants representing the distance travelled over the course of a period. This is a periodic running solution in that over one period the particles each travel a uniform distance, and yet the momentum variables are periodic in the standard sense. Notice that such a solution has a non-zero average velocity. That is

\[ \langle \dot{q}_i \rangle = \frac{1}{T} \int_0^T dt \dot{q}_i(t) = \frac{m_i}{T} \neq 0. \quad (5.24) \]

Thus particle $i$ runs to the right (left) when $m_i > 0$ ($m_i < 0$), for $i = 1, 2$. For the dimer the net transport may be zero if $m_1 + m_2 = 0$, that is $m_1 = -m_2$ and the particles run in a counterpropagating fashion with the same average velocity. However, as will be seen, this solution is not possible.

The main results regarding the character of periodic running solutions are contained in the theorem below.
Theorem 5.1. Given the system of coupled oscillators Eq. (II.1) & Eq. (II.2) with \(\kappa > 0\) and \(\gamma > 0\), and assuming periodic running solutions determined by Eq. (5.23) \& Eq. (5.24), then it holds that

(i) For a period of duration \(T\), both particles run over an equal distance. That is \(m_1 = m_2\);

(ii) No (non-trivial) periodic motion is possible in the absence of time-periodic external modulations, i.e. when the driving amplitudes \(h_1 = h_2 = 0\);

In the special case of equal driving amplitudes \(h_1 = h_2 = h\) the following also holds

(iii) Let \(H(t) = h \sin(\Omega t + \Theta_0)\), with period \(T_0 = 2\pi/\Omega\), represent the external time-periodic driving of the system. For solutions that are frequency-locked to \(H(t)\), it holds that the distance between the particles performs periodic oscillations, i.e.

\[ q_1(t + T) - q_2(t + T) = q_1(t) - q_2(t) \] \hspace{1cm} (5.25)

Moreover, the period \(T\) is determined by

\[ T = 2lT_0 \] \hspace{1cm} (5.26)

for some \(l \in \mathbb{Z}\);

(iv) The coordinates obey

\[ q_1 \left( t + \frac{1}{2}T \right) = q_2(t) + k, \quad q_2 \left( t + \frac{1}{2}T \right) = q_1(t) + k, \] \hspace{1cm} (5.27)

with \(k \in \mathbb{Z} \setminus \{0\}\) and hence

\[ q_i(t + T) = q_i(t) + 2k, \quad i = 1, 2. \] \hspace{1cm} (5.28)
5.2. FEATURES OF TRANSPORT

Proof. Suppose that there exists a period $T$ such that the system Eq. (II.1),(II.2) has a running solution of the form given in Eq. (5.23). Multiplying Eq. (II.1) by $\dot{q}_1$ and Eq. (II.2) by $\dot{q}_2$ and adding the two resulting equations we obtain

\[
\frac{d}{dt} \left[ \frac{1}{2} \dot{q}_1^2 + \frac{1}{2} \dot{q}_2^2 - \frac{1}{2\pi} \cos(2\pi q_1) - \frac{1}{2\pi} \cos(2\pi q_1) + \frac{\kappa}{2} (q_1 - q_2)^2 \right] = - (h_1 \dot{q}_1 + h_2 \dot{q}_2) \sin(\Omega t + \Theta_0) - \gamma (\dot{q}_1^2 + \dot{q}_2^2), \tag{5.29}
\]

where the driving term is of period $T_0 = 2\pi/\Omega$. Integrating over one period, $T$, yields

\[
\int_{(n-1)T}^{nT} d \left[ \frac{1}{2} \dot{q}_1^2 + \frac{1}{2} \dot{q}_2^2 - \frac{1}{2\pi} \cos(2\pi q_1) - \frac{1}{2\pi} \cos(2\pi q_1) + \frac{\kappa}{2} (q_1 - q_2)^2 \right] = - \int_{(n-1)T}^{nT} dt \left[ (h_1 \dot{q}_1 + h_2 \dot{q}_2) \sin(\Omega t + \Theta_0) + \gamma (\dot{q}_1^2 + \dot{q}_2^2) \right]. \tag{5.30}
\]

With the running solution as given in Eq. (5.23) the expression in Eq. (5.30) reduces to

\[
\int_{(n-1)T}^{nT} d \left[ \frac{\kappa}{2} (q_1 - q_2)^2 \right] = - \int_{(n-1)T}^{nT} dt \left[ (h_1 \dot{q}_1 + h_2 \dot{q}_2) \sin(\Omega t + \Theta_0) + \gamma (\dot{q}_1^2(t) + \dot{q}_2^2(t)) \right]. \tag{5.31}
\]

Let the r.h.s. of Eq. (5.31) be denoted by $I_n$,

\[
I_n = - \int_{(n-1)T}^{nT} dt \left[ (h_1 \dot{q}_1 + h_2 \dot{q}_2) \sin(\Omega t + \Theta_0) + \gamma (\dot{q}_1^2(t) + \dot{q}_2^2(t)) \right]. \tag{5.32}
\]

It is possible to find an upper bound for $I_n$. First assume (without loss of generality) that $h_1 > h_2$. Also, taking into account the property in Eq. (5.24) and the sinusoidal nature of the first term, and further ignoring the second negative-definite term under
the integral, it follows that $I_n$ is bounded from above. That is, there exists a constant $C > 0$ such that

$$I_n \leq h_1(|m_1| + |m_2|) = C = \text{const.} \quad (5.33)$$

On the other hand, for the l.h.s. of Eq. (5.31) we derive

$$\Delta\kappa,n = \int_{(n-1)T}^{nT} d \left[ \frac{\kappa}{2} (q_1 - q_2)^2 \right]$$

$$= \frac{\kappa}{2} \left[ (q_1(nT) - q_2(nT))^2 - (q_1((n-1)T) - q_2((n-1)T))^2 \right]$$

$$= \frac{\kappa}{2} \left\{ [(q_1(0) + nm_1) - (q_2(0) + nm_2)]^2 - [(q_1(0) + (n-1)m_1) - (q_2(0) + (n-1)m_2)]^2 \right\}. \quad (5.34)$$

Using the notation $\Delta q(0) = q_1(0) - q_2(0)$ and $\Delta m = m_1 - m_2$ one arrives eventually at

$$\Delta\kappa,n = [2\Delta q(0) + (2n - 1)\Delta m] \Delta m. \quad (5.35)$$

For $\Delta m \neq 0$ the term $\Delta\kappa,n$ grows monotonically with increasing $n$ due to the squared $\Delta m$ term. However, the monotonically increasing term appearing on the l.h.s. in Eq. (5.31) cannot equate with a finite $I_n$ for all $n$. There must be a critical value $n = n_c$ at which the possibility of equality in Eq. (5.31) is excluded. Thus the only case in which $\Delta\kappa,n$ is guaranteed to attain finite values, i.e. becomes $n$-independent, is if $\Delta m = 0$, i.e. $m_1 = m_2$. That is, over any period of duration $T$, if the particles are in a periodic running state they will travel an equal distance. This concludes the proof of statement (i) in the above theorem.

For the proof of part (ii) we note that $\Delta m = 0$ in Eq. (5.35) implies

$$\Delta\kappa,n = \int_{(n-1)T}^{nT} d \left[ \frac{\kappa}{2} (q_1 - q_2)^2 \right] = 0, \quad (5.36)$$
so that due to Eq. (5.31) the following relation is true
\[
\int_{(n-1)T}^{nT} dt \left[ (h_1 \dot{q}_1 + h_2 \dot{q}_2) \sin(\Omega t + \Theta_0) + \gamma (\dot{q}_1^2(t) + \dot{q}_2^2(t)) \right] = 0, \quad (5.37)
\]
which in the absence of the external time-dependent modulation, i.e. \( h_1 = h_2 = 0 \), reduces to the condition
\[
\int_{(n-1)T}^{nT} dt (\dot{q}_1^2(t) + \dot{q}_2^2(t)) = 0. \quad (5.38)
\]
This condition can only be satisfied if \( \dot{q}_1 = \dot{q}_2 = 0, q_1 = \text{const.}, \) and \( q_2 = \text{const.} \) which, however, contradicts the assumption of (non-trivial) periodic solutions. Thus, to obtain periodic solutions both \( h_1 \) and \( h_2 \) cannot be zero which proves part (ii) of the theorem.

Parts (iii) & (iv) require that the driving amplitudes for Eq. (II.1) & Eq. (II.2) are equal; that is \( h_1 = h_2 = h \) giving \( H(t) = h \sin(\Omega t + \Theta_0) \). It is now useful to also introduce the difference and sum coordinates of \( q_1 \) and \( q_2 \). These are
\[
x = q_1 - q_2, \quad y = q_1 + q_2. \quad (5.39)
\]
The corresponding equations of motion expressed in the new variables read as
\[
\ddot{x} = -2\kappa x - \gamma \dot{x} - 2 \sin(\pi x) \cos(\pi y) \equiv f(x, \dot{x}, y) \quad (5.40)
\]
\[
\ddot{y} = -\gamma \dot{y} - 2H(t) - 2 \cos(\pi x) \sin(\pi y) \equiv g(x, y, \dot{y}). \quad (5.41)
\]
First note that Eq. (5.40) contains a harmonic restoring force, a result of coupling between the subsystems, that bounds the motion of the difference variable \( x \). This term is absent from Eq. (5.41). Thus it is not excluded that the particles will undergo unbounded motion, however the distance between the particles will always be finite. Further note that the effects of the time-dependent modulations are manifested in Eq. (5.41) only. This suggests that the sum variable can undergo ongoing rotational
motion triggered by the external modulation of period $T_0$, viz. $H(t) = H(t + T_0)$. Accordingly, periodic solutions $y(t)$ of Eq. (5.41) are supposed to be frequency-locked to (multiples of) the external periodic modulation $H(t)$, and using Eq. (5.23) and the proven result from (i), i.e. $m_1 = m_2 = m$, the periodic running solutions of the sum variable $y(t)$ attain the form

$$y(t + lT_0) = y(t) + 2m, \quad \dot{y}(t + lT_0) = \dot{y}(t), \quad \text{and} \quad l \geq 1. \quad (5.42)$$

Given further the reflection symmetry of the difference equation Eq. (5.40), $x \leftrightarrow -x$, symmetric (limit cycle) oscillations of $x(t)$ around $x = 0$ of some period $T$ with

$$x(t + T) = x(t), \quad \dot{x}(t + T) = \dot{x}(t), \quad (5.43)$$

are facilitated for which the following holds

$$x \left( t + \frac{T}{2} \right) = -x(t), \quad \dot{x} \left( t + \frac{T}{2} \right) = -\dot{x}(t). \quad (5.44)$$

In order that Eq. (5.40) supports solutions obeying the relation Eq. (5.44) its r.h.s., $f(x, \dot{x}, y)$, needs to satisfy the reflection symmetry

$$f \left( x \left( t + \frac{T}{2} \right), \dot{x} \left( t + \frac{T}{2} \right), y \left( t + \frac{T}{2} \right) \right) = -f(x(t), \dot{x}(t), y(t)). \quad (5.45)$$

Taking into account the r.h.s. of Eq. (5.40) this results in the following condition

$$\cos \left[ \pi y \left( t + \frac{T}{2} \right) \right] = \cos \left[ \pi y(t) \right]. \quad (5.46)$$

From Eq. (5.42) we obtain $y(t) = y(t + lT_0) - 2m$ which, after substitution in the r.h.s. of Eq. (5.46) gives

$$\cos \left[ \pi y \left( t + \frac{T}{2} \right) \right] = \cos \left[ \pi y(t + lT_0) \right], \quad (5.47)$$
from which follows the relation between the frequencies of the periodic motions in $x(t)$ and $y(t)$:

$$T = 2l T_0.$$  (5.48)

Using the relation $\cos[\pi y(t + 2l T_0)] = \cos[\pi(y(t) + 2 \cdot 2m)] = \cos[\pi y(t)]$ one readily verifies the validity of the condition

$$f(x(t + T), \dot{x}(t + T), y(t + T)) = f(x(t), \dot{x}(t), y(t)),$$  (5.49)

that has to be satisfied further by the r.h.s of Eq. (5.40) in order to support periodic solutions which comply with Eq. (5.43).

Furthermore, given the relations in Eq. (5.43), (5.44) and Eq. (5.48) it holds that

$$x(t + l T_0) = (-1)^l x(t), \quad \dot{x}(t + l T_0) = (-1)^l \dot{x}(t)$$  (5.50)

for integer $l$. It remains to verify that the expressions Eq. (5.42) and Eq. (5.50) for periodic solutions $x(t), y(t)$, that are frequency-locked to the external time-periodic modulation $H(t)$, leave the r.h.s. of the sum equation Eq. (5.41) invariant. We obtain

$$g(x(t + l T_0), y(t + l T_0), \dot{y}(t + l T_0)) =$$

$$= -\gamma \dot{y}(t + l T_0) - H(t + l T_0) - 2 \cos[\pi x(t + l T_0)] \sin[\pi y(t + l T_0)]$$

$$= -\gamma \dot{y}(t) - H(t) - 2 \cos[\pi(-1)^l x(t)] \sin[\pi(y(t) + 2m)]$$

$$= -\gamma \dot{y}(t) - H(t) - 2 \cos[\pi x(t)] \sin[\pi y(t)]$$

$$\overset{!}{=} g(x(t), y(t), \dot{y}(t)),$$  (5.52)

ensuring invariance which completes the proof of the statement in (iii).

Finally, combining the expressions in Eq. (5.42) and Eq. (5.50) one infers that in the original coordinates the following holds.
\[ q_1(t + l T_0) = q_2(t) + m \]  
\[ q_2(t + l T_0) = q_1(t) + m \]  
\[ q_i(t + 2l T_0) = q_i(t) + 2m, \quad i = 1, 2, \]  

which concludes the proof of part (iv) of the theorem.

\[ \square \]

5.3 Chapter Summary

This chapter has explored, analytically, some important features of the system of equations given by Eq. (II.1) & Eq. (II.2), which describe two linearly coupled, driven and damped pendula. The first part of the chapter was dedicated to a Melnikov type analysis related to homoclinic bifurcations. Beginning with the unperturbed system and adding weak driving, damping, and coupling, it has been possible, using Melnikov’s method, to derive an expression, in terms of the system’s parameters, for a homoclinic bifurcation signalling the onset of chaos. In more detail, in parameter space a bifurcation point related to the first transverse intersections of the stable and unstable manifolds is derived. Such intersections, being of importance for the existence of strange attractors, indicate the presence of chaotic motions in the system.

The second part of this chapter has explored the properties of transport related to the periodic running solutions described by Eq. (5.23). By assuming such a solution it has been possible to deduce important features of transport when the particles are in a periodic running state. Firstly, in such a state the particles will travel an equal distance. Moreover, counterpropagating trajectories are excluded, i.e. the particles must travel in the same direction. Further, non-trivial periodic solutions are impossible without the time-periodic external modulations. That is, all periodic
running solutions must be frequency locked to certain multiples of the external time-periodic modulations.

The next chapter will look at three specific realisations of Eq. (II.1) & Eq. (II.2) which further illustrate the complexity in the system.
The previous chapter analytically explored some of the dynamics of the class of system described by equations Eq. (II.1) & Eq. (II.2). An expression for a homoclinic bifurcation, signalling the onset of chaos, was derived through the perturbational approach of Melnikov. Attention was also given to a particular type of solution, namely the periodic running solution, and its properties.

Although these results have illuminated some important features of the system, there is much that remains illusive. A thorough analytical analysis of such a system is quite often not possible. To this end, a numerical investigation that will complement the results from Chapter 5 will be carried out in this chapter.

In the introduction to Part II the dynamics of the single driven and damped particle were discussed. In particular, it was shown that depending on the parameters, there were different types of attractors that the dynamics eventually settles on. Fig. II.1 shows two possible attractors. One of these is the regular periodic attractor which supports coherent directed transport, and the other is a strange attractor which supports chaotic motion. It should be noted that there may be coexisting regular attractors, supporting directed motion in opposite directions for instance. These regular attractors will each have a corresponding ‘weight’, related to the size of their

*This is also the title of an article by Mateos (2003)
basins of attraction, and it is these weights that are important when it comes to determining the system’s net current.

Returning to the full system, i.e. the coupled system, an interesting question is what happens when two of these attractors are coupled. That is, what happens to the coupled dynamics when the attractor types of the underlying subsystems are varied. The focus of this chapter will be examining, largely through numerical means, three such systems which correspond to subsystems consisting of strange/strange, strange/regular, and finally regular/regular attractors.

### 6.1 Strange vs Strange Attractor (Model Three)

The first example system that will be explored involves the coupling of two oscillators which, in the uncoupled regime, both have trajectories that evolve on strange attractors. In other words, the trajectories could be said to be chaotic. These orbits contribute nothing to the emergence of a directed current, as for the long time average they have zero momentum. For directed transport, and further for a directed current, to emerge in the coupled system the two subsystems have to suppress chaos while working cooperatively to overcome potential barriers.

The system under consideration is

\[
\dot{q}_1 = -\sin(2\pi q_1) - 0.1\dot{q}_1 + 1.3\sin(2.25 t) - \kappa(q_1 - q_2) , \\
\dot{q}_2 = -\sin(2\pi q_2) - 0.1\dot{q}_2 + 1.3\sin(2.25 t) + \kappa(q_1 - q_2) ,
\]

where exact system parameters that will be used here have been inserted into the equations of the motion. They are $\gamma = 0.1$, $h_1 = h_2 = 1.3$, $\Omega = 2.25$, and $\theta_0 = 0$. The parameter representing the coupling strength, $\kappa$, remains unspecified as the dynamics as a function of this parameter will be under investigation here.
Firstly, let us look at the periodic running solutions described by Eq. (5.23). It is clear that in the uncoupled regime, $\kappa = 0$, a periodic running solution is not possible given that both particles have trajectories that evolve on strange attractors. Turning to the coupled regime, notice then that in the case of identical particle motion, or in-phase motion, the particles effectively decouple. Thus the dynamics is determined by two independent oscillators which evolve on strange chaotic attractors. This holds for all values of $\kappa$ showing that transporting in-phase (synchronous) motion supported by a regular periodic attractor is excluded. However, this does not exclude the possibility of a periodic running solution where the two particles have motions that are out of phase. Such a solution can be seen in Fig. 6.1 where the time evolution of the coordinates $q_1, q_2$ is shown, and the coupling strength is chosen as $\kappa = 0.46$. It is apparent that both are frequency locked to the external driving. This is also illustrated in Fig. 6.1 by the inclusion of the function $F(t) = \sin(2.25 t)$ oscillating around $q = 1564$.

Fig. 6.2 shows the same trajectory projected onto the effective potential given by $U(q_1, q_2) = \frac{2 - \cos(2\pi q_1) - \cos(2\pi q_2)}{(2\pi)}$. This figure highlights the cooperation between the particles which allows directed transport to take place. One unit will move backward in order for both units to move forward. In an alternating manner, one unit will sacrifice for the benefit of the dimer.

Importantly, from Fig. 6.1 & Fig. 6.2 it can be deduced that the temporal behaviour of the coordinates follows the relations given in Eqs. (5.25)-(5.28).

### 6.1.1 Influence of the Coupling Strength

Taking as example coupling strengths $\kappa = 0$, where there exist strange attractors for both particles, and $\kappa = 0.46$, where the motion can be periodic, it seems that coupling strength plays a key role for the dynamics of the system. The fact that the system exhibits rich and complex dynamics is expected given that the phase-space is five dimensional. Conversely, the fact that the two chaotic subsystems can combine
Figure 6.1: Time evolution of the coordinates $q_{1,2}(t)$ of the two particles representing a periodic running state being frequency-locked to the external time-periodic modulation. The parameter values are given by $\Omega = 2.25$, $h_1 = h_2 = 1.3$, $\theta_0 = 0$, $\gamma = 0.1$, and $\kappa = 0.46$. For comparison, $\sin(\Omega t)$ oscillating around $q = 1564$ with unit amplitude and frequency $\Omega = 2.25$ is shown (dashed line).

to produce regular periodic motion is less expected. The character of the phase flow evolving in this five-dimensional phase-space is conveniently displayed by a Poincaré map using the period of the external force, $T_0 = 2\pi/\Omega$, as the stroboscopic time. The system of equations of motion was integrated numerically and, after omitting a transient phase, points were set in the map at times being multiples of the period duration $T_0$. In Fig. 6.3 the bifurcation diagram for one of the particles (a qualitatively similar diagram exists for the other particle), as a function of the coupling strength, is depicted.
Figure 6.2: Evolution of the trajectory associated with the two particles in a periodic running states in the spatially periodic potential landscape $U(q_1, q_2)$. The parameter values are the same as in Fig. 6.1.

Figure 6.3: Bifurcation diagram as a function of the coupling strength and remaining parameter values: $\Omega = 2.25$, $h_1 = h_2 = 1.3$, $\theta_0 = 0$, and $\gamma = 0.1$. 
This diagram is largely characterised by windows of chaotic motion which are most prevalent in the range of coupling strengths \(0 \leq \kappa \leq 0.6\). There are however, at least two windows (visible on the scale of the figure) were periodic solutions are permitted, one of which covers almost one sixth of the \(\kappa\) values continuously. This is quite important. Firstly, it confirms that there is a phenomenon in which \textit{chaos combines with chaos to form regular periodic motion}. By this, it is meant that in the uncoupled regime both subsystems support chaotic motion, but in the coupled regime there exist periodic solutions. Secondly, it shows that this phenomena is robust (structurally stable) in that, for the windows of periodic motion, the solutions persist under small changes of the coupling strength.

With regard to the emergence of a non-zero current, the favourable coupling strengths are those that correspond to the periodic windows in the bifurcation diagram. It may be the case though that there are multiple coexisting attractors, each contributing to overall dynamics with a different weight, and it is these weights that determine the strength of the current. These weights can of course be related to the size of the corresponding basins of attraction.

To gain a quantitative perspective on how \(\kappa\) influences the system dynamics we compute the current \(v_m\) as defined in Eq. (2.5). To reiterate, the time averaged mean velocity is computed for an ensemble of initial conditions, which is given by

\[
v_m = \frac{1}{T_s} \int_0^{T_s} dt \left( \frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{2} \dot{q}_{i,n}(t) \right),
\]

with simulation time \(T_s = 10^5\). Here \(N (= 5000)\) denotes the number of initial conditions. These initial conditions are chosen such that the particles have positions \(q_{1,2}(0)\) that are distributed uniformly over one (spatial) period of the corresponding potential (i.e. a single potential well) and randomly chosen velocities \(\dot{q}_{1,2}(0)\) with \(|\dot{q}_{1,2}(0)| \leq 0.5\). This range of velocities has been chosen for the sake of the numerics only. The results remain qualitatively the same for velocities outside of this range.
The results are contained in Fig. 6.4 where the mean velocity is expressed in terms of the ratio of the spatial and temporal periods $L/T_0 \equiv v_0$ with $v_0 \simeq 0.358$ being the velocity of running solutions that advance by one spatial period during one period duration of the external field.

For this range of coupling strengths, $0 \leq \kappa \leq 0.6$, the net current is close to zero, except for a window of $\kappa$-values where the current is non-zero and shows a sensitive dependence on the choice of $\kappa$, viz. changes in the direction of the current. Indeed this window of non-zero net current coincides, as expected, with the large window of periodic motion seen in Fig. 6.3. Regarding the additional windows of periodic motion observed in Fig. 6.3 it is worth noting that there is no directed current for the corresponding coupling strengths. This suggests that there exists symmetry between the coexisting attractors which take trajectories in opposite directions. Thus an equal number of trajectories travel in the range of positive and negative coordinates, i.e. the basins of attraction, promoting motion different directions, are of the same size. This results in a zero current.

**Figure 6.4:** Mean velocity $v_m/v_0$ as a function of the coupling strength and the remaining parameter values are as in Fig. 6.3.
6.2 Strange vs Regular Attractor (Model Four)

Let us consider a different system, similar to the first with the exception that one of the driving amplitudes is altered. Now, rather than have both particles evolve on strange attractors, when in the uncoupled limit $\kappa = 0$, one of these particles will now evolve on a regular periodic attractor. In more detail, $h_1$ is chosen such that the corresponding (uncoupled) particle dynamics are chaotic, while the choice of $h_2$ will allow for regular dynamics. Fig. II.1 shows the resulting attractors for the underlying subsystems. In addition, the figure contains an example trajectory illustrating the system’s uncoupled dynamics. The two dynamical regimes are clearly distinguishable. To achieve directed transport in the coupled system, the subsystem promoting periodic motion must suppress the irregular dynamics of its chaotic counterpart. The system is modelled by the following set of coupled ordinary differential equations

\begin{align*}
\ddot{q}_1 &= -\sin(2\pi q_1) - 0.1\dot{q}_1 + 1.3\sin(2.25t) - \kappa(q_1 - q_2), \\
\ddot{q}_2 &= -\sin(2\pi q_2) - 0.1\dot{q}_2 + 1.5\sin(2.25t) + \kappa(q_1 - q_2),
\end{align*}

where system parameters are $\gamma = 0.1$, $h_1 = 1.3$, $h_2 = 1.5$, $\Omega = 2.25$, and $\theta_0 = 0$. Again, the parameter representing the coupling strength, $\kappa$, will quite often be used as a control parameter, and thus will remain unspecified. Note that the exchange symmetry $(\dot{q}_1, q_1) \leftrightarrow (\dot{q}_2, q_2)$, present in Model Three, is not present in this model – which from now will be called Model Four. This impedes the possibility of synchronisation between the particles as they have different underlying subsystems.

6.2.1 Emergence of a Current

The true complexity of this system is revealed only when the individual units making up the dimer are coupled together, i.e. when $\kappa \neq 0$. To gain a quantitative
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perspective on how $\kappa$ influences the system dynamics we again compute the current $v_m$ as described by Eq. (6.3).

The initial conditions are chosen such that in the uncoupled case one particle’s trajectory lies on the chaotic attractor, and the other on the periodic attractor. In more detail, the initial conditions corresponding to the subsystem with driving force of strength $h_1$ have positions $q_1(0)$ that are distributed uniformly over the (spatial) period of the potential and randomly chosen velocities $\dot{q}_1(0)$ with $|\dot{q}_1(0)| \leq 0.5$. The initial conditions corresponding to the subsystem with driving strength $h_2$ were chosen so that the particle undergoes regular rotational motion to the right. Arbitrarily we chose $q_2 = 0, p_2 = 1.5$ for the entire ensemble.

It is clear that when $\kappa = 0$ there will be a (positive) directed current supplied by the particle associated with the periodic attractor. The particles with trajectories evolving on the chaotic attractor will (if at all), on long time scales, provide a vanishingly small contribution to the current (Hennig et al., 2009b). The key question then is, what happens to the current when the dynamics is in the coupled regime?

For computation of the long-time average, using an ensemble of $N = 5000$ initial conditions, the simulation time interval for each trajectory is taken as $T_s = 10^5$. Further, the current was calculated for 1000 (evenly spaced) values of $\kappa$ in the range $0 \leq \kappa \leq 0.04$. The results are contained in Fig. 6.5.

As expected, for $\kappa = 0$ there is indeed a directed current. With low values of $\kappa$ a number of current reversals (shown on inset in Fig. 6.5), induced by desymmetrisation of the saddles, can be seen (cf. § 4.2-4.3). To be precise the chain of chaotic saddles being arranged along the particle’s path in the washboard potential organise the escape of particles from the potential wells. Due to breaking of the spatial invariance the corresponding invariant stable/unstable manifolds arrange differently with respect to motion to the left and right.

Interestingly, moving from the uncoupled to the coupled regime there is a sudden
Figure 6.5: The current, defined in § 6.2.1, as a function of the coupling strength \( \kappa \). The red (dashed) line serves to highlight the line of zero current. The remaining parameters are \( h_1 = 1.3, h_2 = 1.5, \gamma = 0.1, \) and \( \Omega = 2.25 \). The top inset shows the current for \( \kappa \geq \kappa_c \) and the bottom inset shows the occurrence of current reversals for low coupling values.

Figure 6.6: The four Lyapunov exponents as a function of \( \kappa \). The dashed line serves as a guide to the eye. The remaining parameter values are given in Fig. 6.5. Inset shows the largest Lyapunov exponent for low \( \kappa \) values.
current reversal which, strikingly, sees the magnitude of the current almost double. This increase in magnitude is because the transporting particle is able to drag the non-transporting particle, as illustrated in Fig. 6.7. The inset further shows that motion of the transporting particle remains regular even after being coupled to a second (chaotic) particle. The motion of the non-transporting particle remains chaotic. However, there exist ballistic-like channels, which the particles ‘stick’ to aperiodically, where the motion of this particle appears regular and directed for finite periods of time. After this period of regular (directed) transport, the particle settles back into chaotic motion. This is analogous to the ballistic channels present in non-autonomous Hamiltonian systems (Denisov et al., 2002a). An example of one such period of ballistic-like motion is highlighted by two vertical lines in the inset of Fig. 6.7. When not in this channel the chaotically evolving particle has an average velocity that, at times, is close to zero. However, when the particle enters the ballistic-like channel its average velocity increases to $v_c \approx -1.07$. In contrast, the particle whose motion is always regular has an average velocity of $v_r \approx -0.36$.

Returning to the current, it is seen that in the window $0.001 \lesssim \kappa \lesssim 0.015$ a negative current is supported, followed by a transition to zero. It is this transition and the subsequent negligible current which is of most interest to us. To explain this we will look at the Lyapunov spectrum for the system given by the equations of motion Eqs.(II.1)-(II.2).

The Lyapunov spectrum was computed using the method of Wolf et al. (1985), which allows for the simultaneous estimation of all of the system’s Lyapunov exponents. This involves repeated applications of Gram-Schmidt orthonormalisation to ensure that all vectors do not misalign along the direction of maximal expansion. A similar approach is detailed in Parker & Chua (1989). The results are contained in Fig. 6.6. As was mentioned earlier, the passing from an uncoupled to a coupled regime can be seen to mark the beginning of a competition between two dynamical regimes. With very weak coupling it is the regular dynamics that prevails. Not only can a


Figure 6.7: Example trajectory in the low coupling regime — $\kappa = 0.00008$. The inset shows a magnification of the early evolution of this trajectory. Shown between the vertical lines is a period of ballistic-like motion where the average velocity of the particles is $v_c \approx -1.07$ (shown in blue), and $v_r \approx -0.36$.

directed current be found, but also the effect of chaos is, to an extent, suppressed. Looking more closely at the only positive Lyapunov exponent in this regime (inset Fig. 6.6), we see that when the particles become coupled an instant reduction in the magnitude of the exponent follows. For low values of $\kappa$ the spectrum remains almost constant with one positive and three negative Lyapunov exponents. In the range $0.016 \lesssim \kappa \lesssim 0.024$ two of the exponents diverge from one another. Crucially, this divergence sees one of the exponents approach zero. This divergence also coincides with a reduction in the magnitude of the current (see Fig. 6.5). At a critical coupling value $\kappa_c \approx 0.024$ a second exponent becomes positive marking the transition to, what is known as, hyperchaos. The term hyperchaos was first introduced by Rössler (1979). It represents a highly unstable form of chaotic motion due to exponential growth in more than one phase-space direction. Looking again at Fig. 6.5, it can be seen that at $k_c$ the current is almost negligible. Thus, the transition to hyperchaos (enhancing
unstable motion by adding a further direction of exponential growth) has removed any inherent bias in the system and now no direction of motion is favoured, i.e. the possibility of a directed current is excluded. In the next subsection we will discuss phase-space structures and how they change with increasing $\kappa$, and in addition relate them to the current and Lyapunov spectrum discussed in this subsection.

6.2.2 Phase-Space Structures

We have seen in the uncoupled regime, i.e. non-interacting particles, that it suffices to examine (stroboscopically) the phase-space for each one and a half degree subsystem individually (see Fig. II.1). However, when the particles are coupled the phase-space becomes five dimensional and such representations, yielding four dimensional Poincaré surfaces of section (PSSs), are no longer suitable. We instead will present three dimensional projections of the four dimensional PSSs illustrating the changes in phase-space through increased coupling. Further, for each $\kappa$ there are four possible three dimensional projections that illustrate qualitatively the same point, and thus three of them will be omitted.

Fig. 6.8(a) shows one of the three dimensional projections for the case of weak coupling, $\kappa = 0.01$ (note that the attractors in Fig. 6.8 are coloured with red indicating motion to the left, and blue representing motion to the right). It shows two distinct attractors (each having its own basin of attraction which are separated by impermeable basin boundaries) that take the particles in opposite directions. Strikingly, although these are chaotic attractors, indicated by a positive Lyapunov exponent (cf. previous subsection), the motion on them is nevertheless effectively directed. Like in the uncoupled case, for the subsystem driven at $h_2 = 1.5$, the different weights attached to these transporting attractors favour a directed current (Fig. 6.5), a feature that is maintained up to coupling strengths $\kappa \lesssim 0.016$. We recall that in a single particle system, i.e. $\kappa = 0$, the directed motion results from a lowering of the dynamical symmetry caused by the external modulation field (Yevtushenko et al., 2000;
Hennig et al., 2008). That is, even though the potential and the external driving field are with respect to space and time symmetric respectively, with the choice of a fixed phase $\theta_0$ the symmetry of the flow is reduced and a phase-dependent net motion is found. Due to symmetry reasons it holds that the sign of the mean velocity is reversed upon the changes $\theta_0 = 0 \rightarrow \theta_0 = \pi$ and $h_2 \rightarrow -h_2$ respectively. However, there exists a phase $0 < \theta_0 < \pi$ for which symmetry between the two coexisting periodic attractors, supporting solutions with velocities of opposite sign, $v$ and $-v$, is restored and therefore the net motion vanishes. Hence, in this case for the coupled system the two attractors and their respective basins of attraction are symmetric in phase-space.

As previously mentioned, the transition to a negligible current is an interesting feature of this system (see Fig. 6.5). Relating this to the phase-space, when the coupling strength, playing the role of the bifurcation parameter, is increased the three dimensional projections of the PSSs reveal that the two attractors get larger and eventually merge (cf. Fig. 6.8(b) and Fig. 6.8(c)). That is a merging crisis takes place, for which at a critical value $\kappa_m \approx 0.015$ the two enlarged attractors collide simultaneously with the basin boundary which separate their basins of attraction. As a result they eventually merge, after the crisis, forming a single large chaotic attractor in phase-space (Grebogi et al., 1983; Ott, 1992). Note for the $\kappa_m \approx 0.015$ when the crisis occurs there is only one positive Lyapunov exponent. The beginning of the crisis coincides with the event when two of the Lyapunov exponents diverge from each other, with one of them rapidly approaching zero upon increasing the value of $\kappa$ (corresponding to the green and blue line in Fig. 6.6). At the same time the current rapidly approaches zero. It is also worth noting that if just one of the four three-dimensional projections shows separated attractors, then the attractors are separated in the four-dimensional phase-space. Conversely, to observe a merging of the attractors in the four-dimensional phase-space, it requires that all four three-dimensional projections show a merging of the attractors. This has been observed in
Figure 6.8: Left column: Three dimensional projections of the attractors in phase-space for different coupling strengths. Top: $\kappa = 0.01$, Middle: $\kappa = 0.02$, Bottom: $\kappa = 0.04$. The remaining parameter values are given in Fig. 6.5. The blue (red) points belong to such orbits whose initial conditions are situated in the basin of attraction of a transport-providing attractor. Right column: Examples of corresponding trajectories with the centre of mass shown in green.
Fig. 6.8(b) and Fig. 6.8(c).

Moreover, for under-critical values of $\kappa_m \lesssim \kappa \lesssim \kappa_c$, when the degree of merging is not too pronounced (cf. Fig. 6.8(b)) so that the structure of the formerly separated attractors is still discernible, trajectories jump in a random fashion from the remnant of one of the attractors, after having spent a considerable amount of time there, to the other one and vice versa. As the coupling strength is increased these sojourn times get shorter and shorter. This is illustrated in Fig. 6.8(b), where, as the result of growth and more pronounced merging, the attractor is covering larger regions of phase-space and the associated net current is already very close to zero. The final three dimensional projection Fig. 6.8(c) with $\kappa = 0.04$ shows the phase-space when hyperchaos is well established. In addition, this coupling strength corresponds to a vanishingly small current. The two attractors have now completely merged indicating that no direction of motion is favoured. In other words, symmetry between forward and backward motion is restored. To demonstrate that the attractors have completely merged, we present in Fig. 6.9 all possible two-dimensional projections of the four-dimensional phase-space. The transition of the current to zero taking place in the hyperchaotic regime is illustrated in the top inset in Fig. 6.5 exhibiting a rapidly decaying envelope of the current for $\kappa > \kappa_c$.

The features of the attractors before and after the merging crisis are reflected in the time evolution of the example trajectories displayed in Fig. 6.8. In more detail, for coupling strength $\kappa = 0.01$ the trajectories in the right panel of Fig. 6.8(a) resemble a transporting periodic trajectory of the uncoupled regime. Only a magnification of the plot reveals the chaotic wiggling of the trajectories around the seemingly straight line corresponding to unidirectional particle transport. As the two attractors in phase-space are separated the motion of the particles, associated with a pair of trajectories captured by one of the attractors, proceeds unidirectionally.

In contrast, for coupling strength $\kappa = 0.02$, i.e. after the merging crisis, the pair of trajectories shown in Fig. 6.8(b) undergoes sudden changes in direction belonging
in phase-space to transitions between the ‘skeletons’ of the two attractors having been transporting before the merging crisis. Finally, in the hyperchaotic regime for \( \kappa = 0.04 \) the pair of trajectories exhibits no coherent properties at all (cf. Fig. 6.8(c)). In phase-space there is a single large chaotic attractor left and thus, the ‘skeletons’ of the formerly transporting attractors have completely disappeared.

### 6.3 Regular vs Regular Attractor (Model Five)

The final model that will be considered will consist of, in the uncoupled limit, two subsystems whose underlying attractors promote regular motion. The parameters are chosen such that the individual particles can undergo rotational motion of a directed nature - see Fig. II.1 for a relevant attractor and corresponding example trajectory. In fact, there are coexisting attractors promoting rotational motion to either the left or to the right. The uncoupled particles each have non-zero time-averaged velocity. Thus it is expected, at least in the weak coupling regime, that the current will be non-zero. However, it will be seen that, just as in the strange vs regular attractor model (cf. § 6.2), there exists a range of coupling strengths such that the system supports hyperchaotic motions which coincides with a window of vanishingly small current. That is, rather than work cooperatively to achieve directed transport, here the cooperative effects between the two regular subsystems can act destructively hindering each others progress through the potential landscape.

The system under consideration is

\[
\begin{align*}
\dot{q}_1 &= -\sin(2\pi q_1) - 0.1\dot{q}_1 + 1.5\sin(2.25t) - \kappa(q_1 - q_2), \\
\dot{q}_2 &= -\sin(2\pi q_2) - 0.1\dot{q}_2 + 1.5\sin(2.25t) + \kappa(q_1 - q_2),
\end{align*}
\]

(6.6)

(6.7)

where system parameters are \( \gamma = 0.1, \ h_1 = h_2 = 1.5, \ \Omega = 2.25, \) and \( \theta_0 = 0. \) As
Figure 6.9: All possible two-dimensional projections (excluding reflections) showing the merging of the two attractors for the case $\kappa = 0.04$. The remaining parameter values are given in Fig. 6.5.
before, the parameter representing the coupling strength, $\kappa$, will quite often be used as a control parameter, and thus will be specified only when necessary. Note that the exchange symmetry $(q_1, q_1) \leftrightarrow (q_2, q_2)$ is restored, which was destroyed in Model Four by use of unequal driving amplitudes $h_1 \neq h_2$. This model will now be called Model Five.

### 6.3.1 Current

As before, the current and Lyapunov spectrum have been calculated, as they give insight into the system dynamics for a relevant range of coupling strengths. However, the details of these calculations are omitted as they are contained in the previous sections (cf. § 6.1.1).

Fig. 6.10 shows the current as a function of the coupling strength $\kappa$. This figure is characterised by frequent changes in the direction and magnitude of the current, and an extended window of vanishingly small current. The corresponding Lyapunov spectrum (Fig. 6.11) suggests that when the current is non-zero all of the Lyapunov exponents (excluding the trivial exponent related to the time variable which is always zero) are negative. Conversely, when the current is approximately zero, some of the Lyapunov exponents become positive. In fact, for this system two of the exponents become positive. Thus, in this window of coupling strengths the system exhibits hyperchaos. Further, it appears that, just as in Model Four, hyperchaos (and not chaos with only one positive Lyapunov exponent) is the cause of a vanishingly small current. Evidence in this direction is provided by the fact that Model Four has one positive Lyapunov exponent for the full range of $\kappa$ considered, and yet there is a non-zero current. However, when a second exponent becomes positive, then the current approaches zero.

Also of note is the sharp transition from regular motion to hyperchaos (and also the transition from hyperchaos to regular motion). This transition marks a rapid
Figure 6.10: The particle current, as defined in Eq. (6.3), as a function of the coupling strength $\kappa$, where $h_1 = h_2 = 1.5$. The remaining parameters are given in Fig. II.1. The red dotted line serves as a guide for the eye.

Figure 6.11: The four Lyapunov exponents as a function of $\kappa$, where $h_1 = h_2 = 1.5$. The remaining parameters are given in Fig. II.1. The red dotted line serves as a guide for the eye.
change of the structures in the higher dimensional phase-space. In short, when the motion is regular (no positive Lyapunov exponents) trajectories stick to attractors supporting regular motion. However, at the bifurcation point marking the transition to hyperchaos, invariant manifolds belonging to hyperbolic structures (with access to wider parts of the phase-space) become intertwined with the basins of attraction of the transport supporting attractors. Eventually, trajectories get readily caught in these hyperbolic structures and perform permanent chaotic motion. In a sense, these former regular structures begin to leak. In the previous section a similar transition was related to an attractor merging crisis. Ultimately, porous phase-space structures and an attractor merging crisis have a similar effect on a system’s dynamics. That is, trajectories are no longer confined to certain (transport promoting) regions in phase-space (see Conclusion).

6.4 Chapter Summary

Chapter 6 has been dedicated to a numerical exploration of systems that model linearly coupled driven and damped particles, described by Eq. (II.1) & Eq. (II.2), outside of the perturbational regime. These models are characterised by the attractors of the underlying subsystems when the said subsystems are uncoupled from one another, which have been chosen to be either regular or strange. For each system there exists windows, within the range of coupling considered, for which the current exhibits a sensitive dependence on the strength of the coupling, viz. changes in the direction and/or magnitude of the current. The current reversals observed here, induced by a change in a system parameter, differ from those in Mateos (2003) where the current reversals are related to the basins of attraction for the system’s coexisting attractors that produce counterpropagating motion.

Regarding the system dynamics, two general points have emerged. Firstly, co-
operation between the particles leads to the suppression of the effects of chaos, and can even result in regular periodic motion that facilitates directed transport (see Fig. 6.1). This is evident, particularly in Model Three and Model Four, when one considers the emergence of a non-zero net current in spite of the fact that motion occurs on a strange attractor. The second point to emerge is that the regime of hyperchaos appears to coincide with a non-zero net current. In fact, the transition chaos – hyperchaos (hyperchaos – chaos) marks the transition from a non-zero (zero) current, to a zero (non-zero) current. Interestingly, this effect appears to be a general feature of these systems. However, this requires further examination which is beyond the scope of this thesis (see Conclusion).
Conclusion

Summary

This thesis has considered systems of coupled oscillators, both in the autonomous (Hamiltonian) and nonautonomous (driven and damped) cases, with a view to examining different transport regimes. Through analytical and numerical means the aim has been to develop a thorough understanding of the coupled dynamics in such systems. Of particular interest were the conditions under which directed transport can emerge. Sometimes this is a trivial artefact of the initial conditions (including parameters). Let it be, for example, insufficient energy for the particles to overcome the potential barriers – no transport, and thus no current; or it may be that there is sufficient energy, but the coupling between the particles is weak and the initial direction of motion is maintained – non-zero current. However, quite often it is the case that directed transport can only emerge when the particles work together. That is, cooperative effects become very important. Ultimately, the focus has been on exploring the ensemble behaviour of these systems.

A key point that has been evident throughout this thesis is that cooperation between the particles allows for new transport scenarios that are not permitted in the case of a single particle. Consider two examples, one from Part I, and another from Part II. In Chapter 2 it was observed that a stationary particle is able to escape from its initial confining well and undergo directed transport, after a transient period of chaotic energy exchange with a second particle. If the particles were uncoupled, this
initially stationary particle would remain trapped for all time as this system is free from external perturbations. Therefore, it is cooperation between the particles that allows the initially stationary particle to become transporting. Conversely, the process of permanent bond formation (dimerisation) may result, as a consequence of the coupling, yielding no net transport. With a view to applications, this process may be seen as a filter capturing/blocking a particle by impeding its movement. As a second example, let us turn to Chapter 6 (§ 6.1). For the particular model considered there, if the subsystems are uncoupled, then the dynamics is chaotic with the individual particles evolving on strange attractors. However, when the particles are coupled, it is possible that the motion can become regular and periodic (cf. Fig. 6.1). Thus, working together the particles can suppress the effects of chaos. This effect of suppression of chaos was also observed in § 6.2, where the systems only positive Lyapunov exponent (in the uncoupled limit) decreased almost to zero as a result of coupling between the particles.

Finally, this thesis also examined two different coupling regimes. In Part I the coupling was short range in nature, allowing for the effective decoupling of the particles (through increasing distance between the particles). In contrast, the coupling used in Part II was such that the particles remain coupled even when the distance between them is large. It is worth (briefly) discussing the differences between these regimes.

The conservative Hamiltonian systems of Part I were endowed with an initial (low) energy. Using a long range coupling regime in this case would preclude the unbounded directed motion of a single particle, as the energy would be quickly usurped by the interaction potential. Thus, many of the transport scenarios discussed in Part I would not occur. Therefore, it is preferable to have short range coupling in this case.

For the driven and damped systems of Part II the external driving force can cause the rapid separation of the particles. For short range coupling this results in the particles effectively decoupling after short periods of time, even for relatively strong
coupling strengths. The dynamics in this case are not of great interest. This is not true for long range coupling where the dynamics have proven to be very interesting — as was observed, particularly in Chapter 6.

**Outlook**

While this thesis looked at systems of two coupled oscillators, it is certainly worthwhile to extend these results to similar systems with an arbitrary number of degrees-of-freedom. One of the challenges is to develop (reduction) tools, alternative to the method of Poincaré maps, with which geometrical structures such as invariant hypertori in higher-dimensional phase-spaces can be appropriately visualised. However, this task becomes hopeless rather rapidly with increasing \( N \) (the number of degrees-of-freedom) by consequence of the Froschlé conjecture (Lichtenberg & Lieberman, 1983). Therefore, it is appropriate to have a gradual approach to dimension increase (as suggested by Jung et al. (2010) for the problem of chaotic scattering in higher dimensional systems). Work in this direction has already been carried out (see, for example, Katsanikas & Patsis (2011)) using a technique known as *colour and rotation*, where 3D projections of a 4D space are produced and the fourth dimension is represented by colour. While this approach does provide useful information, it is not applicable to higher dimensional systems.

Furthermore, the transition from regular to chaotic motion in higher-dimensional phase-spaces organised by unstable periodic orbits needs to be investigated. That is in order to gain insight into the transition from stability to complex instability the structure of invariant manifolds associated with unstable periodic orbits needs to be explored. In particular with regard to the emergence of transport scenarios in higher-dimensional phase-spaces, the question of whether the phenomenon of stickiness of chaotic orbits to the vicinity of periodic orbits is exhibited by higher-dimensional dy-
namical systems is of paramount interest. Furthermore, diffusion features in higher dimensional systems entailed by motion along unstable invariant manifolds corresponding to unstable periodic orbits with distinct magnitudes of eigenvalues of the linearised systems merit to be addressed. A question of interest is whether multiple channels supporting diffusive behaviour coexist, or is there one dominant channel that prevails.

In Chapter 6 an interesting effect was observed. Namely, the transition to hyperchaos coincides with the transition to a non-zero net current. Intuitively it would appear that this is a generic feature of the class of system considered in Part II. However, this is by no means certain and requires further exploration, not just of the class of system under consideration, but also of different classes of system. In addition, for these systems the effect of the inclusion of more degrees-of-freedom, with respect to the transitions to hyperchaos and current generation, remains unclear.

In Parts I & II the focus was on how the parameter that regulates the coupling strength effects the dynamics. However, it would be interesting to investigate how changes in the systems other parameters (most notably in Part II) influence the dynamics. For example, varying the driving frequencies in Eq. II.1 & Eq. II.2 may allow for interesting resonance effects leading to further complicated transport scenarios not discussed in this thesis.

Finally, it is worth considering the stochastic counterpart of the systems mentioned above. The introduction of noise to a system affects the dynamics in numerous ways depending on the type of noise and its amplitude. With regard to solutions of a system, particularly periodic solutions, noise can be added to test the solutions stability. However, of interest is the study of how trajectories that are close to a separatrix, which separates bounded from unbounded motion, behave. For example, can those trajectories that are in bounded regions of phase-space (or at a localisation/localisation transition in parameter space) be subsequently kicked, under the influence of noise, into unbounded regions of phase-space. Conversely, for those trajectories in
unbounded regions of phase-space, is noise enhanced trapping (Altmann & Endler, 2010) a feature of the stochastic system.

APPENDIX
APPENDIX A

Derivation of the Separatrix Solution

The simple pendulum consists of two hyperbolic fixed points corresponding to the pendulum facing vertically upward. These fixed points are connected via heteroclinic connections which for the unperturbed pendulum is just the separatrix that separates bounded from unbounded motion. The equation defining the separatrix is derived here.

The Hamiltonian describing the simple pendulum can be written as

\[ H(p, q) = \frac{1}{2}p^2 + \frac{1 - \cos(2\pi q)}{2\pi}, \]

(1.1)

where \( p \) and \( q \) are the canonically conjugated momentum and position, respectively. The hyperbolic fixed points are located at \( (p, q) = (0, \pm 1/2) \). Thus

\[ H\left(0, \pm \frac{1}{2}\right) = \frac{1}{2}(0)^2 + \frac{1 - \cos(\pm\pi)}{2\pi} = \frac{1}{\pi}. \]

(1.2)

Therefore, for the pendulum to leave a regime of libration motion and undergo rotations, it must have energy greater than \( E_s = 1/\pi \). In other words, the curve with energy \( E_s = 1/\pi \) splits the phase space into two distinct regions – that of bounded motion, and that of unbounded motion. Equating this energy to the Hamiltonian gives
\[
\frac{1}{2}p^2 + \frac{1 - \cos(2\pi q)}{2\pi} = \frac{1}{\pi}.
\] (1.3)

Rearranging and using the trigonometric identity \(\cos(2x) = 1 - 2\sin^2(x)\) we obtain

\[
p = \pm \sqrt{\frac{2}{\pi} - \frac{2}{\pi} \sin^2(\pi q)} = \pm \sqrt{\frac{2}{\pi} \cos(\pi q)}. \tag{1.4}
\]

The \(\pm\) is due to the hyperbolic fixed points having a stable and an unstable manifold.

From Hamilton’s equations of motion we have that \(p = \dot{q}\). Thus

\[
\dot{q} = \pm \sqrt{\frac{2}{\pi} \cos(\pi q)}. \tag{1.5}
\]

From which we obtain

\[
\int \frac{dq}{\cos(\pi q)} = \pm \int \sqrt{\frac{2}{\pi}} dt = \pm \sqrt{\frac{2}{\pi}} t. \tag{1.6}
\]

Looking now at the left hand side, and using the substitution \(x = \pi q\), we have

\[
LHS = \frac{1}{\pi} \int \frac{dx}{\cos(x)} = \frac{1}{\pi} \int \sec(x) dx = \frac{1}{\pi} \int \sec(x) \left(\frac{\sec(x) + \tan(x)}{\sec(x) + \tan(x)}\right) dx, \tag{1.7}
\]

\[
LHS = \frac{1}{\pi} \int \frac{\sec^2(x) + \sec(x) \tan(x)}{\sec(x) + \tan(x)} dx. \tag{1.8}
\]

Taking the substitution \(u = \sec(x) + \tan(x)\), Eq. 1.8 reduces to

\[
LHS = \frac{1}{\pi} \int \frac{1}{u} du = \frac{1}{\pi} \ln(u). \tag{1.9}
\]

Now equating left and right hand sides of Eq. 1.6 (also using the substitutions for \(u\) and \(x\)) we have

\[
\ln[\sec(\pi q) + \tan(\pi q)] = \pm \sqrt{2\pi} t, \tag{1.10}
\]

and thus
\[
\sec(\pi q) + \tan(\pi q) = \exp(\pm \sqrt{2\pi} t). \tag{1.11}
\]

Looking just at the left hand side

\[
\sec(\pi q) + \tan(\pi q) = \frac{1}{\cos(\pi q)} + \frac{\sin(\pi q)}{\cos(\pi q)} = \frac{1 + \sin(\pi q)}{\cos(\pi q)}. \tag{1.12}
\]

Squaring the top and bottom gives

\[
\sqrt{\frac{(1 + \sin(\pi q))^2}{\cos^2(\pi q)}} = \sqrt{\frac{(1 + \sin(\pi q))^2}{1 - \sin^2(\pi q)}} = \sqrt{\frac{(1 + \sin(\pi q))^2}{(1 + \sin(\pi q))(1 - \sin(\pi q))}}, \tag{1.13}
\]

which reduces to

\[
\sqrt{\frac{1 + \sin(\pi q)}{1 - \sin(\pi q)}}. \tag{1.14}
\]

Now Eq. 1.11 becomes

\[
\sqrt{\frac{1 + \sin(\pi q)}{1 - \sin(\pi q)}} = \exp(\pm \sqrt{2\pi} t). \tag{1.15}
\]

Squaring both sides gives

\[
\frac{1 + \sin(\pi q)}{1 - \sin(\pi q)} = \exp(\pm 2\sqrt{2\pi} t). \tag{1.16}
\]

To be concise, let \( S = \sin(\pi q) \) and \( E = \exp(\pm 2\sqrt{2\pi} t) \). Eq. 1.16 now looks like

\[
\frac{1 + S}{1 - S} = E. \tag{1.17}
\]

Therefore

\[
1 + S = E(1 - S) = E - ES. \tag{1.18}
\]

Rearranging

\[
S + ES = E - 1. \tag{1.19}
\]
Therefore

\[ S = \frac{E - 1}{E + 1}. \]  

(1.20)

That is

\[ \sin(\pi q) = \frac{\exp(\pm 2\sqrt{2\pi} t) - 1}{\exp(\pm 2\sqrt{2\pi} t) + 1}. \]  

(1.21)

Using the trigonometric identity

\[ \tanh(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)} = \frac{\exp(2x) - 1}{\exp(2x) + 1}. \]  

(1.22)

Eq. 1.21 becomes

\[ \sin(\pi q) = \tanh(\pm \sqrt{2\pi} t) \]  

(1.23)

Finally we obtain

\[ q^\pm = \frac{1}{\pi} \sin^{-1} \left( \tanh(\pm \sqrt{2\pi} t) \right) \]  

(1.24)

In the unstable direction \( q^+(t) \)

\[ \lim_{t \to +\infty} q^+(t) = \frac{1}{\pi} \sin^{-1}(1) = \frac{1}{\pi} \frac{\pi}{2} = \frac{1}{2}, \]  

(1.25)

while

\[ \lim_{t \to -\infty} q^+(t) = \frac{1}{\pi} \sin^{-1}(-1) = \frac{1}{\pi} \frac{\pi}{2} = -\frac{1}{2}, \]  

(1.26)

as expected. The same analysis can be applied to the stable direction \( q^-(t) \).

Now let \( t = x/\sqrt{2\pi} \), from which we obtain \( dt = dx/\sqrt{2\pi} \). Then

\[ p^\pm = \dot{q}^\pm = \frac{1}{\pi} \frac{d}{dt} \sin^{-1}(\tanh(\pm \sqrt{2\pi} t)) \]  

(1.27)
becomes

$$p^\pm = \frac{\sqrt{2}}{\sqrt{\pi}} \frac{d}{dx} \sin^{-1}(\tanh(\pm x))$$  \hspace{1cm} (1.28)

Note

$$\left[ \frac{d}{dx} \sin^{-1}(x) = \frac{1}{\sqrt{1 - x^2}} \right]$$  \hspace{1cm} (1.29)

Therefore

$$p^\pm = \frac{\sqrt{2}}{\sqrt{\pi}} \frac{1}{\sqrt{1 - \tanh^2(\pm x)}} \frac{d}{dx} \tanh(\pm x)$$  \hspace{1cm} (1.30)

As \( \frac{d}{dx} \tanh(x) = \text{sech}^2(x) \), and using the identity \( 1 - \tanh(x) = \text{sech}^2(x) \), Eq. 1.30 becomes

$$p^\pm = \frac{\sqrt{2}}{\sqrt{\pi}} \text{sech}(\pm x) = \frac{\sqrt{2}}{\sqrt{\pi}} \text{sech}(\pm \sqrt{2\pi t})$$  \hspace{1cm} (1.31)

As before, examining the unstable direction \( p^+(t) \), we have

$$\lim_{t \to +\infty} p^+(t) = 0,$$  \hspace{1cm} (1.32)

while

$$\lim_{t \to -\infty} p^+(t) = 0,$$  \hspace{1cm} (1.33)

as expected. The same analysis applies to stable direction \( p^-(t) \). This completes the derivation of the separatrix solution for an unperturbed pendulum.


BIBLIOGRAPHY


