

EXIT CYCLING FOR THE VAN DER POL OSCILLATOR AND QUASIPOTENTIAL CALCULATIONS

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ABSTRACT. We discuss the phenomenon of cycling for noise induced escape to a unstable periodic orbit. The presence of cycling is shown to follow from qualitative properties of two quasipotential functions. A method of numerically evaluating these quasipotential functions is described, and applied to the Van der Pol oscillator as an example. Figures resulting from these calculations reveal that nonconvergent cycling of exit measures does occur for the Van der Pol example.

§1: INTRODUCTION

The Van der Pol equation

$$(1.1) \quad \ddot{y} + \mu(y^2 - 1)\dot{y} + y = 0$$

is a favorite example of a nonlinear system having a unique stable (for $\mu > 0$) periodic solution. In the conventional reduction to a first order system, $x = (x_1, x_2) = (y, \dot{y})$, this becomes

$$(1.2) \quad \dot{x}(t) = \mathbf{b}(x(t)) \quad \text{where} \quad \mathbf{b}(x) = \begin{bmatrix} x_2 \\ -\mu(x_1^2 - 1)x_2 - x_1 \end{bmatrix}.$$

We are going to consider $\mu < 0$ (which is equivalent to reversing time for $\mu > 0$). This makes (1.2) a system with a stable critical point at the origin, surrounded by an unstable limit cycle.

The effects of adding an asymptotically small random perturbation to such a system have been discussed in recent work, such as [2] and other references cited there. Specifically we compare the solution $x(\cdot)$ of (1.2), with initial condition $x(0) = x_0$, to the solution $x^\epsilon(t)$ of the following Itô equation:

$$(1.3) \quad dx^\epsilon(t) = \mathbf{b}(x^\epsilon(t)) dt + \epsilon^{1/2} d\omega(t), \quad x^\epsilon(0) = x_0.$$

The parameter $\epsilon > 0$ is viewed as the strength of the random perturbation. Our interest is in asymptotic behavior as $\epsilon \downarrow 0$. It can be shown in several ways that $x^\epsilon(t) \rightarrow x(t)$ uniformly (in probability) over t in any fixed time interval $[0, T]$. The story is different however when we look at the whole time axis, $t \in [0, \infty)$. Let D be the region enclosed by the limit cycle of (1.2), with ∂D being the limit cycle itself. For any $x_0 \in D$ the solution $x(t)$ of (1.2) remains forever in D and converges to 0 as $t \rightarrow \infty$. In contrast to this, $x^\epsilon(t)$ will eventually (with probability 1) wander out to ∂D , reaching it first at some random time $\tau < \infty$. A particularly interesting phenomena occurs in the study of the distribution μ^ϵ of this point $x^\epsilon(\tau)$ of first "noise induced" escape to the limit cycle ∂D :

$$(1.4) \quad \mu^\epsilon(A) = P[x^\epsilon(\tau) \in A], \quad A \subseteq \partial D.$$

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One might expect μ^ϵ to converge, as $\epsilon \downarrow 0$, to some limiting probability measure on ∂D . However the theory suggests that such convergence will hold only in very rare examples. The typical behavior is what we call *periodic cycling*. If we could watch the probability measure μ^ϵ on ∂D change as ϵ is decreased to 0 we would see it precess or cycle around ∂D , roughly as if it was being transported along by the flow of (1.2), with $\log(\epsilon^{-1/2})$ as the elapsed time. This cycle will (asymptotically) repeat itself each time $\log(\epsilon^{-1/2})$ advances by one period of the limit cycle. [2] presents this more precisely, and explains why this will result in the failure of μ^ϵ to converge, except in rare examples. One goal of this paper is to offer numerical evidence that (nonconvergent) periodic cycling of μ^ϵ does occur for the Van der Pol system (1.3) in particular.

We will not exhibit cycling of μ^ϵ through direct simulations or numerical calculations. Rather we numerically evaluate two specific functions whose properties are linked to the behavior of μ^ϵ by the mathematical theory. These two functions are the quasipotential $V(\cdot)$ (famous from the work of Wentzell and Freidlin [6]) and the boundary quasipotential $W(\cdot)$. In Section 2 we will briefly introduce these two functions and present Theorem 1, which explains how the phenomenon of nonconvergent cycling is manifest in qualitative properties of V and W . Then, in Section 3, we will discuss some figures which exhibit graphically these qualitative features, allowing us to invoke Theorem 1 for the example (1.3).

The remainder of the paper concerns the justification of Sections 2 and 3. Section 4 explains the numerical calculations used to obtain the figures in Section 3, and the theoretical basis of these calculations. Section 5 is devoted to proving Theorem 1. Both of these sections depend heavily on detailed understanding of V and W culled from earlier work, [4] and [3].

The significance of the quasipotential functions (Theorem 1) and our method of evaluating them numerically (Section 4) are not peculiar to the Van der Pol example. Our discussion applies to any example satisfying the following hypotheses, which are assumed throughout the paper. $x^\epsilon(t)$ is the (2-dimensional) solution of

$$(1.5) \quad dx^\epsilon(t) = \mathbf{b}(x^\epsilon)dt + \epsilon^{1/2}\sigma(x^\epsilon)d\omega(t), \quad x^\epsilon(0) = x_0 \in D.$$

($\omega(t)$ is a standard 2-dimensional Wiener process and (1.5) is taken in the Itô sense.) The vector field $\mathbf{b}(\cdot)$ and nonsingular 2×2 matrix function $\sigma(\cdot)$ are smooth on \mathbb{R}^2 . (We take smooth to mean C^∞ . This is simply to avoid chasing degrees of differentiability through our discussion; C^n for $n \approx 3$ would probably be enough.) The origin is an asymptotically stable critical point of

$$(1.6) \quad \dot{x}(t) = \mathbf{b}(x(t)),$$

with all eigenvalues of $B = \frac{\partial \mathbf{b}}{\partial x}(0)$ having negative real parts. The origin is surrounded by an unstable limit cycle, with characteristic multiplier $m_1 > 1$. D denotes the region enclosed by the limit cycle, so that ∂D is the limit cycle itself. We assume that D contains no other critical points or periodic orbits of (1.6); for every $x(0) \in D$ the corresponding solution $x(t)$ of (1.6) has $x(t) \in D$ for all $t > 0$ with $x(t) \rightarrow 0$ as $t \rightarrow +\infty$. The perturbed Van der Pol system (1.3) is the particular case with \mathbf{b} as in (1.2) and $\sigma(\cdot) \equiv I$.

The exit measure μ^ϵ is as defined in (1.4). The dependence on x_0 is suppressed in the notation because this dependence does not influence any of the results described below; the reader may take $x_0 = 0$ in the definition of μ^ϵ .

It may be worth observing that certain “storage functions” of interest in nonlinear H_∞ control have much of the same structure as our quasipotential functions; see [5] and [1]. Thus the numerical approach described here may also be useful in exploring examples from that context.

§2: QUASIPOTENTIAL FUNCTIONS AND CYCLING

The two quasipotential functions, $V(\cdot)$ and $W(\cdot)$, are central to our discussion. Theorem 1 below links them to the asymptotic behavior of μ^ϵ . They are defined in terms of the “probabilistic action” of Wentzell and Freidlin. For an absolutely continuous $\phi : [0, T] \rightarrow \mathbb{R}^2$ define

$$S_{0T}(\phi) = \int_0^T L(\phi, \dot{\phi}) dt$$

where the Lagrangian L is given by

$$L(x, \mathbf{v}) = \frac{1}{2}(\mathbf{v} - \mathbf{b}(x))^T a(x)^{-1}(\mathbf{v} - \mathbf{b}(x)).$$

The matrix $a(x)$ is obtained from the $\sigma(x)$ of (1.5):

$$a(x) = \sigma(x)\sigma(x)^T.$$

It is therefore smooth, symmetric and positive definite. $S_{0T}(\phi)$ measures (in a sense made precise by large deviations theory) how unlikely it is for $x^\epsilon(t)$ to follow the path $\phi(t)$, for $0 \leq t \leq T$.

The original *quasipotential* function is defined in \bar{D} (the closure of D) by

$$(2.1) \quad V(x) = \inf S_{0T}(\phi),$$

where the infimum is over all $T > 0$ and absolutely continuous paths $\phi : [0, T] \rightarrow \bar{D}$ with $\phi(0) = 0$ and $\phi(T) = x$. In some sense $V(x)$ measures the probabilistic difficulty of going from $x^\epsilon(0) = 0$ to $x^\epsilon(t) = x$ at some $0 < t < \infty$ without leaving \bar{D} first.

The *boundary quasipotential* function is defined in \bar{D} by

$$W(x) = \inf S_{0T}(\phi)$$

where this time the infimum is over all $T > 0$ and absolutely continuous $\phi : [0, T] \rightarrow \bar{D}$ with $\phi(0) = x$ and $\phi(T) \in \partial D$. It measures the probabilistic difficulty of completing an exit to ∂D from y .

Properties of V and W have been studied in [4] and [3] respectively. They are both nonnegative continuous functions in \bar{D} . $V(0) = 0$ with $V > 0$ in $\bar{D} \setminus \{0\}$. $W = 0$ on ∂D with $W > 0$ in the interior of D . More of their structure will be detailed in section 4 in order to explain how we have computed them numerically. The point here is that nonconvergent cycling of the exit distribution μ^ϵ can be deduced from qualitative features of V and W . Theorem 2 and its corollary in Section 5 provide equivalent conditions which can help identify the presence of these features. Here we use a description in terms of level sets, i.e. sets of the form

$$\{x \in D : V(x) = c_V\} \quad \text{and} \quad \{x \in D : W(x) = c_W\},$$

for constants c_V and c_W . We say the level sets of V are *coincident* with the levels sets of W if for every c_V there is a c_W such that the two level sets agree, and likewise for every c_W there is a c_V .

Theorem 1. *If the level sets of V are not coincident with the level sets of W then μ^ϵ exhibits nonconvergent cycling as $\epsilon \downarrow 0$.*

The proof of Theorem 1 is discussed in section 5 below. Here we offer the following rough heuristic explanation. Consider a level set C of W : $C = \{W = w_0\}$ for some $w_0 > 0$. (If w_0 is sufficiently small C will be close to ∂D where W is known to be smooth, hence references to $dW = [\frac{\partial W}{\partial x_1}, \frac{\partial W}{\partial x_2}]$ below can be justified.) Since $W(y)$ is constant over $y \in C$, the difficulty of completing an exit to ∂D from y is the same for all $y \in C$. Hence among all possible exit ‘‘routes’’ from 0 to ∂D the most likely ones are those which pass through those points $y^* \in C$ which are most easily reached from 0, namely those $y^* \in C$ at which V is minimal: $V(y^*) \leq V(y)$, all $y \in C$. If the V and W level sets do not coincide then the set C^* of such y^* is a proper subset of C . It turns out that from a given $y \in C$ the most likely way to complete an exit to ∂D is to follow

$$(2.2) \quad \dot{x} = \mathbf{b}(x) - dW(x)^T; \quad x(t_0) = y$$

for roughly $\log(\epsilon^{-1/2})$ time units and then exit to a nearby boundary point:

$$x^\epsilon(\tau) \approx x(\log(\epsilon^{-1/2}) + t_0).$$

Now ∂D is a stable limit cycle for (2.2). So if the y^* form a proper subset C^* of C then we see the distribution μ^ϵ of $x^\epsilon(\tau)$ concentrated around $x(\log(\epsilon^{-1/2}) + t_0)$ only for those solutions of (2.2) with $x(t_0) \in C^*$. These $x(\log(\epsilon^{-1/2}) + t_0)$ approximate a proper subset of ∂D , which cycles or precesses around ∂D periodically in $\log(\epsilon^{-1/2})$, producing the nonconvergent cycling.

§3: LEVEL SETS FOR THE VAN DER POL SYSTEM

The four accompanying figures show some of the V and W level sets for the Van der Pol system (1.3) using two parameter values: $\mu = -1$ and $\mu = -2$. We discuss the latter of these first, since the significant features are more easy to discern in that case. In all figures the dotted lines indicate V levels, while solid lines are used for W levels and the limit cycle ∂D itself.

The Case of $\mu = -2$.

Figure 1 shows ∂D (the outer curve) enclosing V and W level sets corresponding to the values indicated in. The $W = .005$ set is solid line closest to ∂D , with the higher W levels being farther into the interior. $V = .005$ is the small ellipse near the center; the larger V levels are the concentric dotted curves surrounding it. Looking carefully, we can see the $V = .6$ level crossing and recrossing the $W = .6$ level in both the first and third quadrants.

Figure 2 is an enlarged view showing the crossing of V and W levels in the first quadrant more clearly. Clearly the $V = .6$ level set does not coincide with a W level, and hence by Theorem 1 nonconvergent cycling must occur for this example.

The Case of $\mu = -1$.

Figure 3 shows the limit cycle for $\mu = -1$ with an assortment of V and W levels. In this case the V and W levels seem to be rather close in shape. However differences between $V = .35$ and $W = .5$ are visible with close scrutiny.

Figure 4 is an enlargement, using a selection of levels which reveals the noncoincidence more clearly. $W = .5$ is close to $V = .375$ at the top left but crosses $V = .35$ in the lower right. The $V = .2$ and $W = .75$ levels can also be seen to cross. Again we find the noncoincidence of the V and W levels to be apparent.

The Fins.

The reader will notice the sharp fin-shaped extrusions attached to some of the W level sets: $W \geq .1$ for $\mu = -2$, $W \geq .75$ for $\mu = -1$. Figure 2 affords the clearest view. These fins are not actually part of the indicated level set, such as $\{W = .5\}$ in Figure 2, but are an artifact of our computational approach. (See Section 4.) The presence of these fins *is* significant however. The “cross point” where the fin joins the level set proper is a nonsmooth point for the quasipotential function. The presence of fins on either the V or W levels implies the V levels are not coincident with the W levels, as we will explain in Section 5. Hence the existence of fins in our pictures is another sufficient condition for nonconvergent cycling.

§4: COMPUTATION OF QUASIPOTENTIALS

The numerical calculations used to obtain the graphs of the preceding section will be explained here. While we make no claims of numerical efficiency for our approach, it is solidly founded on detailed analysis of $V(\cdot)$ and $W(\cdot)$, which we summarize below. First we describe some notation and conventions.

The collection of “spatial” points $x \in \mathbb{R}^2$ is called *state space*. Many different coordinate systems can be used to represent points in state space – we will have to deal with a nonstandard one in our discussion of W below. Until then however we can limit ourselves to the conventional cartesian coordinates x_1, x_2 and consider all quantities to be defined in terms of coefficients with respect to them. For purposes of expressions in which a state x occurs as a factor in a matrix product we will view it as a column matrix: $x = [x_1, x_2]^T$. Likewise vectors are taken as columns:

$$\dot{x} = \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix}, \quad \mathbf{b}(x) = \begin{bmatrix} u_1(x_1, x_2) \\ u_2(x_1, x_2) \end{bmatrix}.$$

The $u_i(x_1, x_2)$ are the specific functions which define the dynamical system (1.6). (1.2) gives them expressly for the Van der Pol system. We write

$$\frac{\partial \mathbf{b}}{\partial x} = \begin{bmatrix} \frac{\partial u_i}{\partial x_j} \end{bmatrix}$$

for the matrix of partial derivatives.

The p variables below are taken as rows $p = [p_1, p_2]$ in matrix product expressions. For such a p and a vector $\mathbf{v} = [v_1, v_2]^T$, we use $\langle p, \mathbf{v} \rangle$ to denote the scalar

$$\langle p, \mathbf{v} \rangle = p_1 v_1 + p_2 v_2.$$

Figure 1: $\mu=-2$

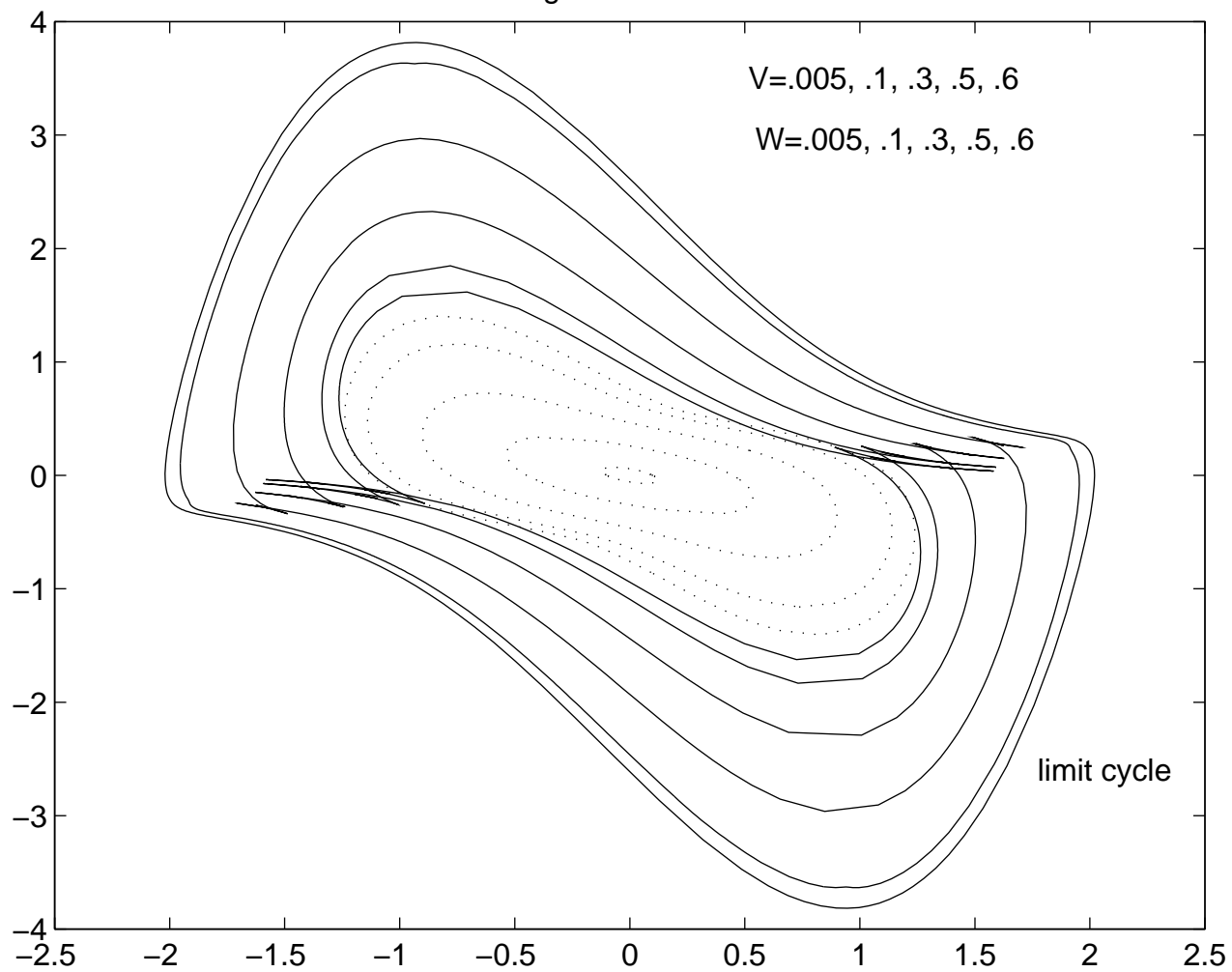


Figure 2: $\mu=-2$

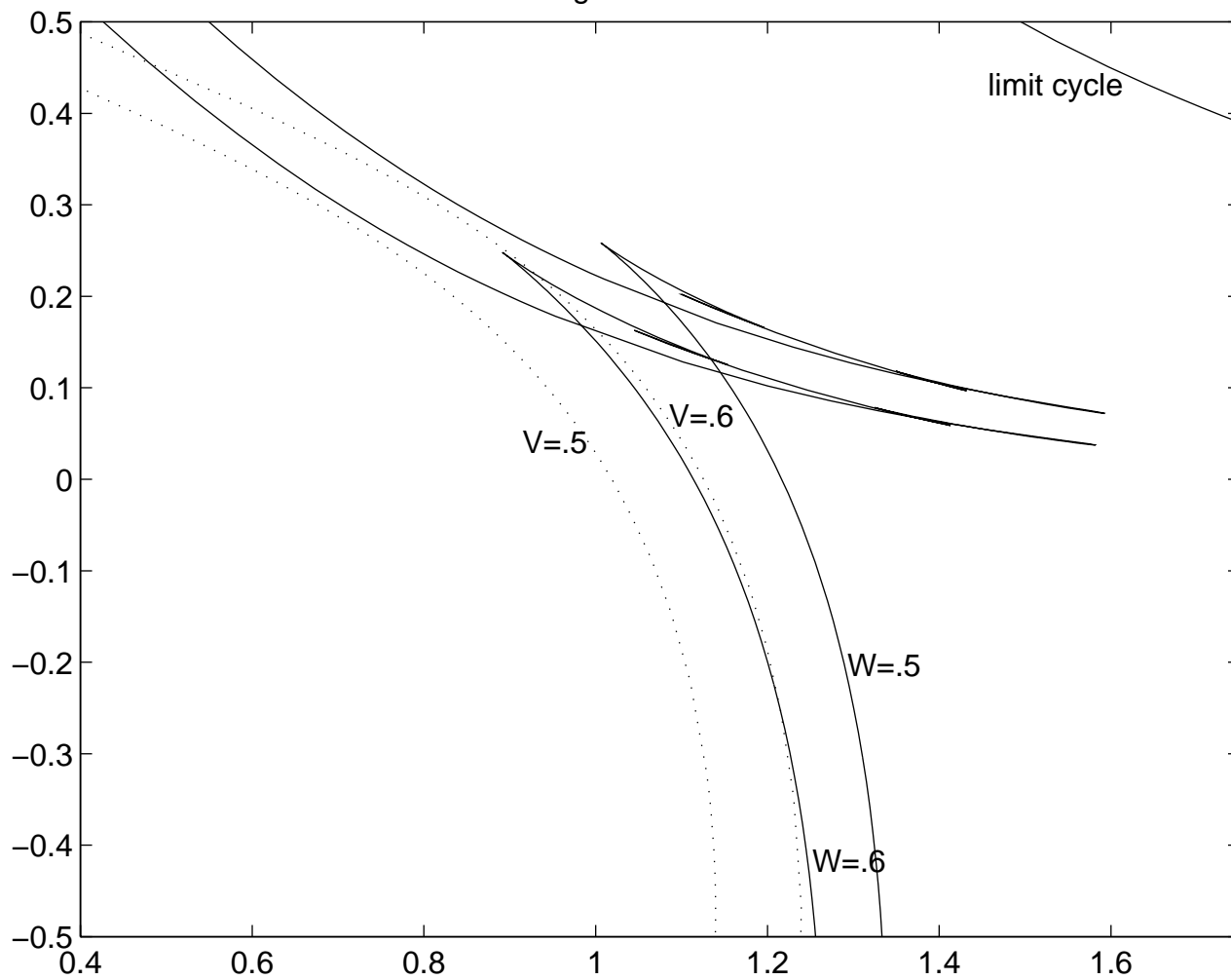


Figure 3: $\mu=-1$

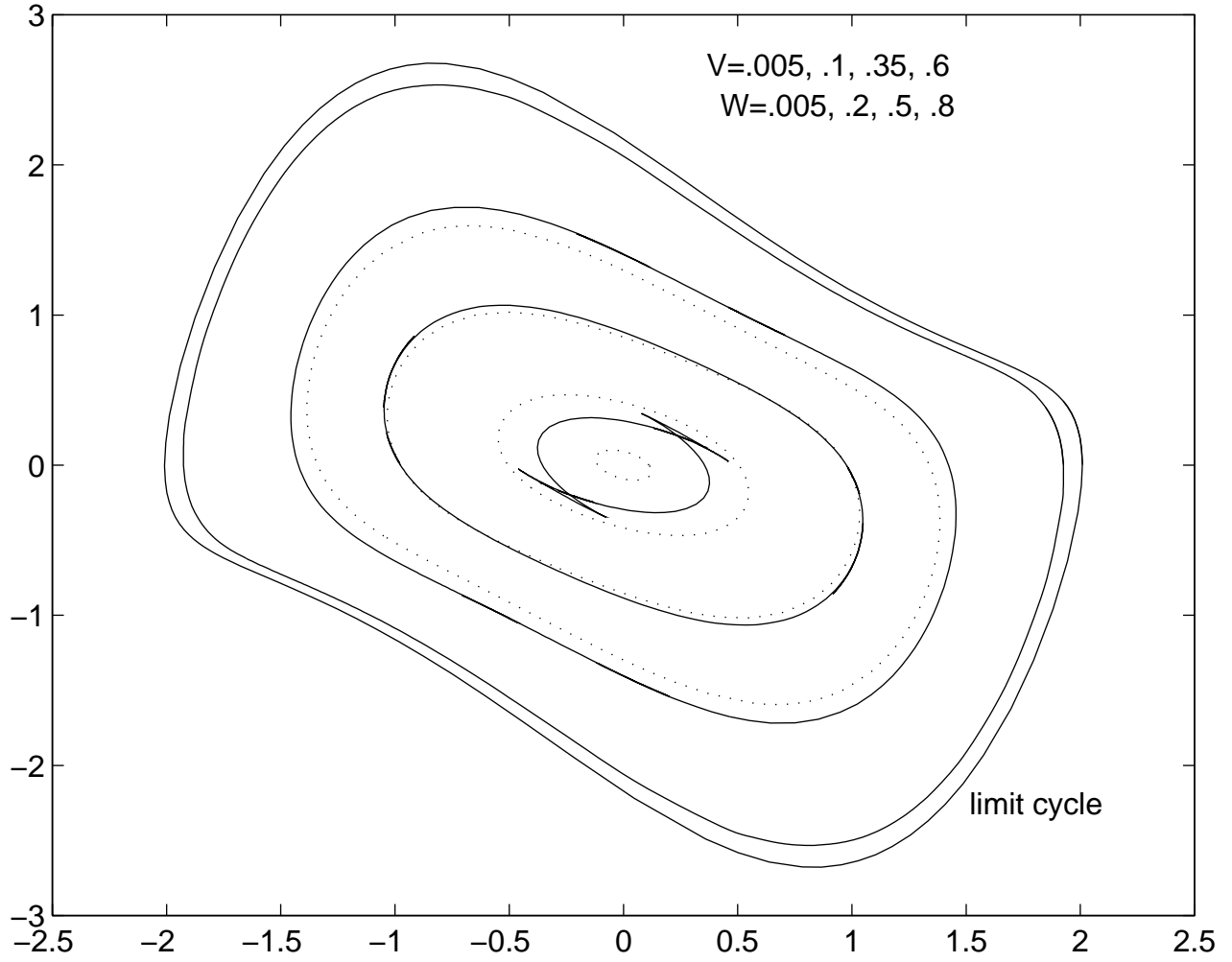
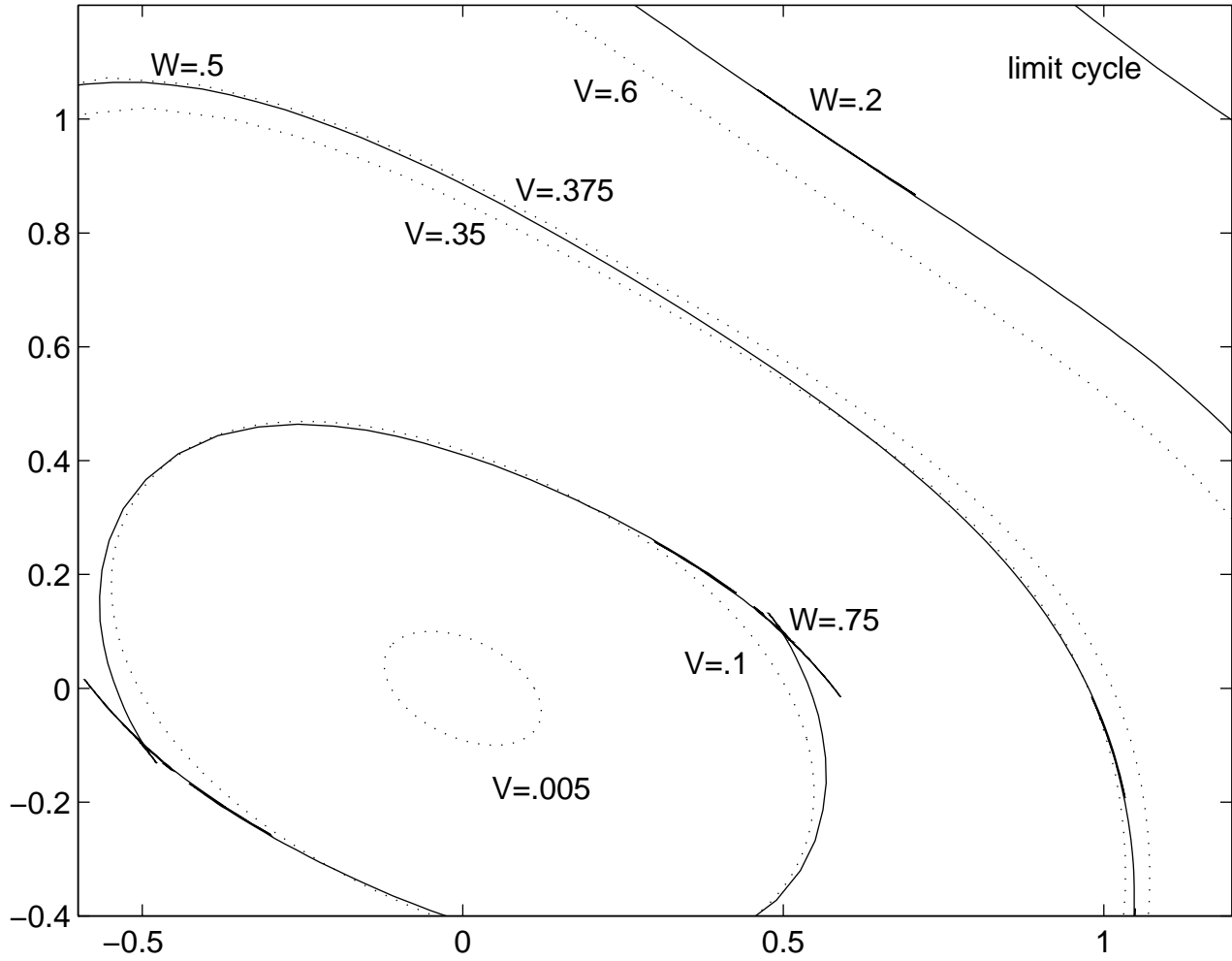


Figure 4: $\mu=-1$



If $V(\cdot)$ is differentiable at a point x then $dV(x) = [\frac{\partial V(x)}{\partial x_1}, \frac{\partial V(x)}{\partial x_2}]$ denotes the row of partial derivatives. This is appropriate since $dV(x)$ will often provide the value of p in what follows.

We will work with the Hamiltonian

$$H(x, p) = \frac{1}{2} \langle p, a(x)p^T \rangle + \langle p, \mathbf{b}(x) \rangle.$$

(According to the above conventions $a(x)p^T$ defines a (column) vector, so that $\langle p, a(x)p^T \rangle$ makes sense.) $H(x, \cdot)$ is the convex dual of $L(x, \cdot)$:

$$(4.1) \quad L(x, \mathbf{v}) \geq \langle p, \mathbf{v} \rangle - H(x, p),$$

with equality for $\mathbf{v} = H_p(x, p) = \mathbf{b}(x) + a(x)p^T$. The Hamiltonian system associated with H is

$$(4.2) \quad \dot{x}_i = H_{p_i}(x, p), \quad \dot{p}_i = -H_{x_i}(x, p).$$

The x equations of (4.2) can be written as

$$\dot{x} = \mathbf{b}(x) + a(x)p^T.$$

The p equations are more complicated since they involve second derivatives of \mathbf{b} . One can check that for any solution of (4.2),

$$(4.3) \quad p_i = L_{v_i}(x, \dot{x})$$

and

$$(4.4) \quad L(x, \dot{x}) = \frac{1}{2} \langle p, a(x)p^T \rangle.$$

The collection of (x, p) is called *phase space*. The Hamiltonian system (4.2) is a first order system of differential equations in phase space. A solution $x(t), p(t)$ of (4.2) is called a *bicharacteristic* and its trajectory in phase space,

$$\{(x(t), p(t)) : t \in \mathbb{R}\},$$

is called a *phase path* or *phase trajectory*. Note that (4.2) is autonomous; a solution can be translated in time to produce a new solution $x(\cdot + c), p(\cdot + c)$ but which traces the same trajectory. We will write $h_t(\cdot, \cdot)$ for the flow associated with (4.2). I.e. if $x(\cdot), p(\cdot)$ solves (4.2) then

$$(x(t), p(t)) = h_t(x(0), p(0)).$$

Note that while vectors in state space are two dimensional, vectors in phase space are four dimensional, denoted $[X_1, X_2, P_1, P_2]^T$ below.

Quasipotential.

Some basic properties of the quasipotential V are deduced directly from its definition (2.1). We have already mentioned that V is continuous in \bar{D} , $V(0) = 0$, and $V(x) > 0$ if $x \neq 0$. The fact that ∂D is a periodic orbit of (1.6) implies that V is constant over ∂D :

$$V(x) = v_{\partial D} \quad \text{for all } x \in \partial D.$$

Although the upper bound $V \leq v_{\partial D}$ is valid throughout \bar{D} , it is possible that $V(x) = v_{\partial D}$ at some interior points x as well as on the boundary.

Our computation of V exploits the intimate connection of V with the Hamiltonian system (4.2), as developed in [4]. For those $y \in D$ with $V(y) < v_{\partial D}$ there exists what we call a *V-minimizing bicharacteristic to y*: a solution $x(\cdot), p(\cdot)$ to (4.2) which passes through $y = x(t_0)$ at some t_0 and satisfies

$$\begin{aligned} x(t) &\rightarrow 0 \quad \text{as } t \rightarrow -\infty, \\ H(x(t), p(t)) &\equiv 0 \end{aligned}$$

and

$$V(y) = V(x(t_0)) = \int_{-\infty}^{t_0} \frac{1}{2} \langle p(t), a(x(t))p(t)^T \rangle dt.$$

In light of (4.4) we can interpret the above as saying $x(\cdot)$ achieves the infimum defining $V(y)$ but using a semi-infinite time interval $(-\infty, t_0]$ instead of a bounded $[0, T]$. We hasten to point out that $x(\cdot), p(\cdot)$ will necessarily achieve the minimum to all $x(t)$ for $t < t_0$ as well,

$$(4.5) \quad V(x(t)) = \int_{-\infty}^t \frac{1}{2} \langle p, a(x)p^T \rangle,$$

but this can fail if $t > t_0$ is sufficiently large. In fact for each V -minimizing bicharacteristic there exists $\tau \in (-\infty, \infty]$ so that $x(\cdot), p(\cdot)$ is minimizing to $x(t)$ for $t \leq \tau$ but not for $t > \tau$. Moreover $V(\cdot)$ is smooth in a neighborhood of each of the $x(t)$, $t < \tau$ and $p(t) = dV(x(t))$ there, a fact we will use in the next section.

Observe that $x = 0, p = 0$ is a critical point for (4.2). It turns out that the V -minimizing bicharacteristics are precisely those lying on the unstable manifold \mathcal{M}_0 for that critical point. I.e. \mathcal{M}_0 is the union of the trajectories of all V -minimizing bicharacteristics. The $x(t), p(t)$ for $t > \tau$ are still considered part of \mathcal{M}_0 , even though the minimum to $y = x(t)$ may be achieved by a different $\tilde{x}(\cdot), \tilde{p}(\cdot)$ to $y = \tilde{x}(s)$. (It must be that $p(t) \neq \tilde{p}(s)$, else the two bicharacteristics would only differ by a translation.)

Another result from [4] says that V is a smooth solution of

$$H(x, dV(x)) = 0$$

in some neighborhood of 0. To be explicit we can take this neighborhood to be

$$N_0 = \{x \in D : V(x) < \delta_0\}$$

for a sufficiently small $0 < \delta_0 < v_{\partial D}$. The manifold \mathcal{M}_0 includes all (x, p) with $x \in N_0$ and $p = dV(x)$. Given a V -minimizing bicharacteristic there is a well-defined first time that $x(t)$ leaves N_0 :

$$\tau_0 = \inf\{t : x(t) \notin N_0\} > -\infty.$$

It is a fact that

$$(4.6) \quad \text{both } x(t) \in N_0 \text{ and } p(t) = dV(x(t)) \text{ hold if and only if } t < \tau_0.$$

It may be that $x(t)$ returns to N_0 at some future time, $t > \tau_0$, but then $p(t) \neq dV(x(t))$ and will have ceased to be V -minimizing, i.e. $t > \tau$.

Consider any $y \in D$ with $V(y) < v_{\partial D}$. There exists at least one (possibly many) bicharacteristics from \mathcal{M}_0 with $x(t) = y$ (some t). For all of these

$$V(y) \leq \int_{-\infty}^t \frac{1}{2} \langle p, a(x)p^T \rangle.$$

Equality will hold for at least one. To find the level set $\{V(x) = c\}$ for a value $0 < c < v_{\partial D}$ we can look at the set of all $x(t_c)$ where $x(\cdot), p(\cdot)$ ranges over the bicharacteristics from \mathcal{M}_0 and t_c is determined by $c = \int_{-\infty}^{t_c} \frac{1}{2} \langle p, a(x)p^T \rangle$. This set will include the level set of V , and possibly some extraneous points coming from those bicharacteristics for which $\tau < t_c$; i.e. which are on \mathcal{M}_0 but are *not* minimizing to $x(t_c)$: $V(x(t_c)) < c$. These extraneous points appear as the ‘‘fins’’ mentioned in Section 3. (Actually no fins are visible on the particular V levels pictured in Section 3. What we observed there were fins on the W levels; see below.)

The system (4.2), with

$$(4.7) \quad \dot{v} = \frac{1}{2} \langle p, a(x)p^T \rangle$$

adjoined can be integrated numerically from an initial point (x_0, p_0, v_0) with $x_0 \in N_0$, $p_0 = dV(x_0)$ and $v_0 = V(x_0)$ to produce a bicharacteristic $x(\cdot), p(\cdot)$ from \mathcal{M}_0 , with $v(t) = V(x(t))$ holding for $t < \tau$. The difficulty is that the only such initial point we know directly is $x_0 = 0, p_0 = dV(0) = 0$, which is a stationary point for (4.2). However the fact that \mathcal{M}_0 is the unstable manifold of (4.2) allows us to compute its tangent space at the critical point $x = 0, p = 0$ and use that to approximate nearby x_0, p_0 on \mathcal{M}_0 . Calculation of the tangent space by linearization of (4.2) was carried out in [4]. Let

$$B = \frac{d\mathbf{b}}{dx}(0), \quad A = a(0).$$

For the Van der Pol example in particular,

$$B = \begin{bmatrix} 0 & 1 \\ -1 & \mu \end{bmatrix}, \quad A = I.$$

The linearization of (4.2) at $x = 0, p = 0$ is

$$\frac{d}{dt} \begin{bmatrix} X_1 \\ X_2 \\ P_1 \\ P_2 \end{bmatrix} = \Lambda \begin{bmatrix} X_1 \\ X_2 \\ P_1 \\ P_2 \end{bmatrix} \quad \text{where } \Lambda = \begin{bmatrix} B & A \\ 0 & -B^T \end{bmatrix}.$$

One invariant subspace for Λ is described by $P_1 = P_2 = 0$, within which the eigenvalues of Λ are just those of B , which are negative. Another (and the one we want) is described by $[X_1, X_2]^T = S[P_1, P_2]^T$ where S is the symmetric 2×2 matrix solving

$$(4.8) \quad BS + A + SB^T = 0.$$

Within this subspace Λ has the same eigenvalues as $-B^T$, which are positive. This means that the tangent space to \mathcal{M}_0 at $x = p = 0$ is given by

$$\begin{bmatrix} P_1 \\ P_2 \end{bmatrix} = S^{-1} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}.$$

We can solve (4.8) explicitly for the Van der Pol example:

$$S = - \begin{bmatrix} \frac{1}{\mu} + \frac{\mu}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{\mu} \end{bmatrix}, \quad S^{-1} = \frac{1}{\frac{1}{\mu^2} + \frac{1}{4}} \begin{bmatrix} \frac{-1}{\mu} & \frac{1}{2} \\ \frac{1}{2} & -(\frac{1}{\mu} + \frac{1}{4}) \end{bmatrix}.$$

Thus we can describe \mathcal{M}_0 and V for $x \sim 0$ by

$$(4.9) \quad p^T = S^{-1}x + o(|x|), \quad V(x) = \frac{1}{2}x^T S^{-1}x + o(|x|^2).$$

Computation. We begin the computation of level sets of V by choosing a small value $0 < v_0$ (we used $v_0 = .005$) and use (4.9) to approximate x and p coordinates of points on \mathcal{M}_0 corresponding to $V(x) = v_0$. Given a unit vector

$$z = [\cos(\theta), \sin(\theta)]^T$$

we take $x_0 = h \cdot z$ where $h > 0$ is chosen so that

$$v_0 = \frac{1}{2}x_0^T S^{-1}x_0 = \frac{1}{2}h^2 z^T S^{-1}z, \quad \text{that is } h = \left(\frac{2v_0}{z^T S^{-1}z} \right)^{1/2}.$$

Then we take $p_0^T = hS^{-1}z$. Doing this for a large selection of $\theta \in [0, 2\pi)$ gives a collection of x_0 approximating the initial level set $\{V(x) = v_0\}$ and the associated $p_0 = dV(x_0)$ in \mathcal{M}_0 . Each of these provides an initial point for (4.2) and (4.9).

Next we select a set of desired V -levels: $v_0 < v_1 < v_2 < \dots < v_n$. For each initial point above we integrate (4.2) and (4.7) numerically, stopping at those times that $v(t_i) = v_i$ and recording the point $x(t_i)$. Thus for each initial point we generate one (possible) point on each of the level sets $\{V(x) = v_i\}$. These sets of points are then plotted, resulting in the figures of the preceding section.

The initial points are only approximations to \mathcal{M}_0 , but because \mathcal{M}_0 is the unstable manifold we expect solutions of (4.2) close to \mathcal{M}_0 to converge to the solutions actually on it. In other words we expect the error in using the linear approximation to \mathcal{M}_0 to be compensated by the negative eigenvalues of Λ , at least initially. We have also checked the sensitivity to this approximation by reducing v_0 to compare with a more accurate approximation. We found negligible differences (on the magnitude scale visible in the figures), thus supporting our confidence in the accuracy of the results.

Boundary Quasipotential.

Most of what has been said about V has an analogue for W ; see [3]. W is continuous in \bar{D} , has $W = 0$ on ∂D and satisfies

$$0 < W(x) \leq W(0) \quad \text{for } x \in D.$$

For any y with $W(y) < W(0)$, the infimum defining $W(y)$ is achieved by some W -minimizing bicharacteristic from y : a solution $x(\cdot), p(\cdot)$ of (4.2) with $x(t_1) = y$, $x(t) \rightarrow \partial D$ as $t \rightarrow +\infty$ (this only means $\text{dist}(x(t), \partial D) \rightarrow 0$, not that $x(t)$ converges to a point on ∂D) satisfying $H(x(t), p(t)) \equiv 0$ and

$$W(y) = \int_{t_1}^{\infty} \frac{1}{2} \langle p, a(x)p^T \rangle dt.$$

There will exist $-\infty \leq \tau^* < \infty$ such that $x(\cdot), p(\cdot)$ is W -minimizing from $x(t)$ for all $t \geq \tau^*$ but not from $x(t)$ for $t < \tau^*$.

The union of the phase trajectories for the W -minimizing bicharacteristics forms a set $\mathcal{M}_{\partial D}$ in phase space which is the stable manifold associated with the periodic solution of (4.2) consisting of the original limit cycle $x(\cdot) \in \partial D$ of (1.6) with $p(\cdot) \equiv 0$ adjoined. W is a smooth solution of $H(x, -dW(x)) = 0$ in a neighborhood

$$N_{\partial D} = \{x \in D : W(x) < \delta_1\}$$

of ∂D . $\mathcal{M}_{\partial D}$ contains the graph of $p = -dW(x)$ for $x \in N_{\partial D}$. For every W -minimizing bicharacteristic,

$$(4.10) \quad \text{both } x(t) \in N_{\partial D} \text{ and } p(t) = -dW(x(t)) \text{ hold if and only if } \tau_1 < t,$$

where τ_1 is the last time $x(t)$ enters $N_{\partial D}$:

$$\tau_1 = \sup\{t : x(t) \notin N_{\partial D}\} < +\infty.$$

Our approach to computing a level set $\{W(x) = c\}$ is analogous to what we did for V . The desired level set will be contained in the set of all $x(t_c)$ where $x(\cdot), p(\cdot)$ range over all the bicharacteristics in the $\mathcal{M}_{\partial D}$ family and t_c is determined by

$$c = \int_{t_c}^{\infty} \frac{1}{2} \langle p, a(x)p^T \rangle dt.$$

This set of $x(t_c)$ may contain extraneous “fins” coming from bicharacteristics for which t_c precedes the time τ^* from which point on $x(\cdot)$ is W -minimizing. (We saw several examples of such fins in Section 3.) We want to carry this out numerically by approximating x_0, p_0 on $\mathcal{M}_{\partial D}$ for which (4.10) holds, and corresponding $w_0 = W(x_0)$, and then integrating (4.2) along with

$$(4.11) \quad \dot{w} = -\frac{1}{2} \langle p, a(x)p^T \rangle$$

backwards in time. We use the tangent space(s) to $\mathcal{M}_{\partial D}$ along ∂D , $p = 0$ to approximate (x_0, p_0) values. These tangent spaces were described in [3]. However that description was in terms of a special boundary coordinate system, not the standard cartesian coordinates x_1, x_2 . Hence we have a number of issues of translation between coordinate systems to work out in order to produce the approximate initial points that we desire.

The boundary coordinate system from [3] identifies points near ∂D using a pair of coordinates denoted ξ_1, ξ_2 . (In [3] x_i denoted the boundary coordinates; we have changed to ξ_i since we are using x_i for cartesian coordinates.) ∂D consists of those points with $\xi_1 = 0$, so that ξ_2 is a parameter along ∂D . To be specific we choose ξ_2 to correspond to units of time along the limit cycle: take $y^*(t)$ to be the periodic solution of (1.6) and identify $\xi_2 = t$. For a given ξ_2 the point with $\xi_1 = 0$ is just $y^*(\xi_2)$. Points with $\xi_1 > 0$ are interior to D on the line normal to ∂D through $y^*(\xi_2)$. Let J be the rotation matrix

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

then

$$J\mathbf{b}(y^*) = \begin{bmatrix} u_2(y^*) \\ -u_1(y^*) \end{bmatrix}$$

is an interior normal to D at $y^* \in \partial D$. (This assumes y^* traverses ∂D in the clockwise direction, the clockwise rotation of \mathbf{b} points into the interior. For counterclockwise rotation of ∂D we would negate the definition of J .) The coordinate map $(\xi_1, \xi_2) \mapsto (x_1, x_2)$ is given explicitly by

$$(4.12) \quad (x_1, x_2) = y^*(\xi_2) + \xi_1 \cdot J\mathbf{b}(y^*(\xi_2)).$$

This formula tells us how to calculate the cartesian coordinates of a point from its boundary coordinates.

We will use both $x = (x_1, x_2)$ and $\xi = (\xi_1, \xi_2)$ to refer to a common point in state space, choosing between the x or ξ notations to emphasize which of the coordinate systems or representations have in mind. For instance $\mathbf{b}(\xi)$ in (4.15) below is the same vector (in the intrinsic sense) as $\mathbf{b}(x)$, but represented differently. We continue to use matrix representations with respect to cartesian coordinates for most formulas of this section; $\mathbf{b} = [u_1, u_2]^T$ and $\frac{\partial \mathbf{b}}{\partial x} = \left[\frac{\partial u_i}{\partial x_j} \right]$ just as above in our discussion of V . Likewise $|\mathbf{b}|^2$ below refers to $(u_1)^2 + (u_2)^2$. Even though we are calculating quantities associated with the boundary coordinate system, we want to be able to carry out the calculations in terms of cartesian representations since that is the form in which we know \mathbf{b} explicitly.

The matrix of partial derivatives (Jacobian) of the coordinate transformation is computed directly from (4.12):

$$(4.13) \quad \frac{\partial x}{\partial \xi} = \begin{bmatrix} \partial x_i \\ \partial \xi_j \end{bmatrix} = [J\mathbf{b} \quad \mathbf{b}] + \xi_1 \cdot [0 \quad J \frac{\partial \mathbf{b}}{\partial x} \mathbf{b}],$$

where the terms from \mathbf{b} and its derivatives on the right are evaluated at $y^*(\xi_2)$. At points $y^*(\xi_2)$ on ∂D ($\xi_1 = 0$) we obtain the matrix of partial derivatives of the inverse coordinate map $(x_1, x_2) \mapsto (\xi_1, \xi_2)$ by a simple inversion:

$$(4.14) \quad \frac{\partial \xi}{\partial x} = \begin{bmatrix} \partial \xi_i \\ \partial x_j \end{bmatrix} = \begin{bmatrix} \partial x_i \\ \partial \xi_j \end{bmatrix}^{-1} = \frac{1}{|\mathbf{b}|^2} \begin{bmatrix} -\mathbf{b}^T J \\ \mathbf{b}^T \end{bmatrix}.$$

The correct ways to translate the representations of state space vectors, p -variables and phase space vectors are guided by the intrinsic understanding of these quantities, i.e. their appropriate mathematical meanings apart from any particular coordinate system. What makes the resulting translation formulas “correct” is that when all quantities are re-expressed in terms of the new representations, $x = (\xi_1, \xi_2)$, $p = [q_1, q_2]$ and $H(\cdot, \cdot) = H(\xi_i, q_i)$, then the Hamiltonian system (4.2) takes the same form in the new expression as it did in the old:

$$\dot{\xi}_i = H_{q_i}(\xi, q), \quad \dot{q}_i = -H_{\xi_i}(\xi, q).$$

The standard intrinsic meaning of a vector at a point is as a first order differential operator with evaluation at the point. Suppose $x = (x_1, x_2)$ and $\xi = (\xi_1, \xi_2)$ are the two coordinate representations of a common point. When functions are expressed in terms of the cartesian coordinates $f(\cdot) = f(x_1, x_2)$ then the action of $\mathbf{b}(x)$ on smooth functions is described by

$$\mathbf{b}(x) = u_1(x_1, x_2)\partial_{x_1} + u_2(x_1, x_2)\partial_{x_2}.$$

The coefficient functions $u_i(x_1, x_2)$ are expressly known to us from (1.6). However if functions are expressed in terms of the boundary coordinates $f(\cdot) = f(\xi_1, \xi_2)$ then the same action of $\mathbf{b}(x) = \mathbf{b}(\xi)$ is expressed

$$(4.15) \quad \mathbf{b}(\xi) = \nu_1(\xi_1, \xi_2)\partial_{\xi_1} + \nu_2(\xi_1, \xi_2)\partial_{\xi_2}$$

using different coefficient functions $\nu_i(\xi_1, \xi_2)$. It follows then that the correct translation formula is

$$(4.16) \quad \frac{\partial x}{\partial \xi} \begin{bmatrix} \nu_1 \\ \nu_2 \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}.$$

Of course the terms are evaluated at the appropriate coordinates ξ_i or x_i of a *common point*.

The construction of our boundary coordinate system implies that the coefficient functions ν_i have a particular asymptotic form near ∂D . Since ∂D is $\{\xi_1 = 0\}$ and \mathbf{b} is tangent to ∂D there, we must have $\nu_1(0, \xi_2) = 0$. This means that

$$\nu_1(\xi) = \xi_1 b_1(\xi) + o(\xi_1)$$

for $\xi_1 \sim 0$, for some function $b_1(\xi)$. Our identification of ξ_2 with time for the motion of (1.6) along ∂D forces $\nu_2(0, \xi_2) = 1$ and so

$$\nu_2(\xi) = 1 + \xi_1 b_2(\xi) + o(\xi_1)$$

for some function $b_2(\xi)$. We will need to evaluate b_1 on ∂D in our numerical calculations. To that end we seek a formula for $b_1(\xi)$ in terms of the cartesian representation of \mathbf{b} , valid on ∂D . Begin with the observation that

$$b_i(\xi) = \partial_{\xi_1} \nu_i|_{\xi_1=0}.$$

Differentiating with respect to ξ_1 in (4.16) gives

$$\begin{bmatrix} \partial_{\xi_1} u_1 \\ \partial_{\xi_1} u_2 \end{bmatrix} = \frac{\partial x}{\partial \xi} \begin{bmatrix} \partial_{\xi_1} \nu_1 \\ \partial_{\xi_1} \nu_2 \end{bmatrix} + \partial_{\xi_1} \frac{\partial x}{\partial \xi} \begin{bmatrix} \nu_1 \\ \nu_2 \end{bmatrix}.$$

Now the left side is

$$\partial_{\xi_1} \mathbf{b} = \frac{\partial \mathbf{b}}{\partial x} J \mathbf{b}.$$

Moreover (4.13) implies that

$$\partial_{\xi_1} \frac{\partial x}{\partial \xi}|_{\xi_1=0} = [0 \quad | \quad J \frac{\partial \mathbf{b}}{\partial x} \mathbf{b}].$$

Using these and our observation that $\partial_{\xi_1} \nu_i = b_i$ on ∂D , we find that

$$\frac{\partial \mathbf{b}}{\partial x} J \mathbf{b} = \frac{\partial x}{\partial \xi} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} + \nu_2 \cdot J \frac{\partial \mathbf{b}}{\partial x} \mathbf{b}.$$

Since $\nu_2 = 1$ on ∂D , we can solve this to obtain

$$\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \frac{\partial \xi}{\partial x} \left[\frac{\partial \mathbf{b}}{\partial x} J - J \frac{\partial \mathbf{b}}{\partial x} \right] \mathbf{b}.$$

From (4.14) and $J^T = -J$ we lift out the formula

$$(4.17) \quad b_1 = \frac{1}{|\mathbf{b}|^2} \mathbf{b}^T \left[J^T \frac{\partial \mathbf{b}}{\partial x} J - \frac{\partial \mathbf{b}}{\partial x} \right] \mathbf{b}.$$

The intrinsic understanding of the p variable is *not* as a vector but rather as a ‘‘covector’’; i.e. it is understood as a linear function acting on vectors. If \mathbf{v} is a vector then the action of p on \mathbf{v} is the intrinsic meaning of the $\langle \cdot, \cdot \rangle$ notation:

$$p : \mathbf{v} \mapsto \langle p, \mathbf{v} \rangle.$$

If $p = [p_1, p_2]$ and $\mathbf{v} = [v_1, v_2]^T$ are the representations with respect to cartesian coordinates then we compute according to the formula

$$\langle p, \mathbf{v} \rangle = p_1 v_1 + p_2 v_2.$$

If we switch to the boundary coordinate representation of the same quantities, $p = [q_1, q_2]$ and $\mathbf{v} = [\mu_1, \mu_2]^T$ and want the same quantity to be evaluated using

$$\langle p, \mathbf{v} \rangle = q_1 \mu_1 + q_2 \mu_2.$$

Then the translation formula (4.16) for vector representations dictates the formula for covector representations:

$$(4.18) \quad \begin{aligned} [p_1, p_2] \frac{\partial x}{\partial \xi} &= [q_1, q_2], \quad \text{or} \\ [p_1, p_2] &= [q_1, q_2] \frac{\partial \xi}{\partial x}. \end{aligned}$$

In particular, our convention of taking $dW(x) = [\frac{\partial W}{\partial x_1}, \frac{\partial W}{\partial x_2}]$ as a covector (row matrix), leads to the correct translation formula (namely the chain rule):

$$dW(x) = dW(\xi) \frac{\partial \xi}{\partial x}.$$

The matrix $a(x)$ acts as a linear map from covectors to vectors, described in coordinates using a matrix product:

$$p \mapsto a(x)p^T.$$

Thus a change in coordinate system will dictate a change in the representation of $a(x)$ as a matrix. If $a(x) = [a_{ij}(x)]$ is the matrix representation for calculation with respect to cartesian coordinate representations, then the matrix representation for boundary coordinate representations would have to be

$$[a_{ij}(\xi)] = \frac{\partial \xi}{\partial x} a(x) \left(\frac{\partial \xi}{\partial x} \right)^T.$$

Our numerical calculations will require evaluation of $a_{11}(\xi)$ on ∂D . From the preceding, $a_{11}(\xi) = d\xi_1(x) a(x) d\xi_1^T(x)$. On ∂D (4.14) tells us that $d\xi_1 = -\frac{1}{|\mathbf{b}|^2} \mathbf{b}^T J$. Thus at a boundary point $(0, \xi_2) = y^*(\xi_2)$ we have the formula

$$(4.19) \quad a_{11} = \frac{1}{|\mathbf{b}|^4} \mathbf{b}^T J a J^T \mathbf{b}.$$

In the Van der Pol example (where $a(x) \equiv I$) this reduces to $a_{11} = \frac{1}{|\mathbf{b}|^2}$.

Points in phase space now have two different coordinate representations: (x_i, p_i) or (ξ_i, q_i) . (4.12) and (4.18) together provide the coordinate map $(\xi_i, q_i) \mapsto (x_i, p_i)$. Vectors in phase space have two corresponding representations:

$$(4.20) \quad X_1 \partial_{x_1} + X_2 \partial_{x_2} + P_1 \partial_{p_1} + P_2 \partial_{p_2} \quad \text{or} \quad \Xi_1 \partial_{\xi_1} + \Xi_2 \partial_{\xi_2} + Q_1 \partial_{q_1} + Q_2 \partial_{q_2}.$$

The conversion is described by

$$(4.21) \quad \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \frac{\partial x}{\partial \xi} \begin{bmatrix} \Xi_1 \\ \Xi_2 \end{bmatrix},$$

since $\frac{\partial x_i}{\partial q_j} = 0$, and

$$[P_1, P_2] = [Q_1, Q_2] \frac{\partial \xi}{\partial x} + [q_1, q_2] D,$$

where

$$D = \sum_i \Xi_i \partial_{\xi_i} \frac{\partial \xi}{\partial x}.$$

At points $(0, \xi_2) \in \partial D$, with $q_i = 0$ this simplifies to

$$(4.22) \quad [P_1, P_2] = [Q_1, Q_2] \frac{\partial \xi}{\partial x}$$

with $\frac{\partial \xi}{\partial x}$ given explicitly by (4.14).

The tangent vectors to $\mathcal{M}_{\partial D}$ at the point $y \in \partial D$, $q = 0$ were shown in [3] to be given (in boundary coordinate representation) by

$$(4.23) \quad Q_1 = \frac{-1}{U(y)} \Xi_1, \quad Q_2 = 0, \quad \Xi_i = \text{arbitrary.}$$

The function U is the unique positive continuous function on ∂D which satisfies

$$(4.24) \quad \frac{d}{dt} U(y^*(t)) = 2b_1 U - a_{11},$$

where b_1 and a_{11} are the functions on ∂D from (4.17) and (4.19). The terms on the right are evaluated at $y^*(t)$. Note that the periodic solution of (4.24) is unstable in forward time, because if ℓ is the period of the limit cycle $y^*(\cdot) \in \partial D$ then $\int_0^\ell b_1(y^*) = \log m_1 > 0$ is its Floquet exponent. However in reverse time the general solution is

$$u(t) = e^{-\int_t^0 2b_1(y^*)} u(0) + \int_t^0 e^{-\int_t^s 2b_1(y^*)} a_{11}(y^*(s)) ds.$$

Hence it is clear that as $t \downarrow -\infty$ all solutions converge to

$$U(y^*(t)) = \int_t^\infty e^{-\int_t^s 2b_1(y^*)} a_{11}(y^*(s)) ds.$$

Given that we know the value of $U(y)$ at a boundary point $y \in \partial D$, the tangent vectors (4.23) to $\mathcal{M}_{\partial D}$ at that point translate to the cartesian representation

$$(4.25) \quad [P_1, P_2] = \left[\frac{-\Xi_1}{U(y)}, 0 \right] \frac{\partial \xi}{\partial x} = \frac{\Xi_1}{U(y) |\mathbf{b}|^2} \mathbf{b}^T J$$

and

$$(4.26) \quad \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \frac{\partial x}{\partial \xi} \begin{bmatrix} \Xi_1 \\ \Xi_2 \end{bmatrix} = \Xi_1 \cdot J \mathbf{b} + \Xi_2 \cdot \mathbf{b}.$$

The manifold $\mathcal{M}_{\partial D}$ is, for (ξ_1, ξ_2) near ∂D , i.e. for $\xi_1 \sim 0$, the graph (in phase space) of $-dW$. In boundary coordinates this means

$$q_i = \partial_{\xi_i} W.$$

The formula (4.23) means that for $(\xi, q) \in \mathcal{M}_{\partial D}$ with $\xi_1 \rightarrow 0$ and $(0, \xi_2) = y \in \partial D$

$$q_1 = \partial_{\xi_1} W(\xi) \sim \frac{\xi_1}{U(y)} \quad \text{and} \quad q_2 = \partial_{\xi_2} W(\xi) \sim 0.$$

This implies

$$(4.27) \quad W(\xi) \sim \frac{\xi_1^2}{2U(y)}.$$

Computation. The first stage of our calculation of W is to locate the limit cycle ∂D and calculate the function U defined on it. We start with an initial guess $x_1(0)$, $x_2(0)$ and $U(0)$ and integrate (1.2) along with

$$(4.28) \quad \dot{U} = 2b_1(x)U - a_{11}(x)$$

backwards in time. (4.17) and (4.19) are used to evaluate the coefficient functions. After a few periods the solution will have converged to the periodic $y^*(t)$ on ∂D and corresponding values of $U(t) = U(y^*(t))$ along it. This produces a large collection of $y^* \in \partial D$ and the corresponding values of $U(y^*)$.

Next we take a small $w_0 > 0$ (such as $w_0 = .005$) and for each known value y^* with $p = 0$ move in the direction specified by tangent vector (4.25), (4.26) with $\Xi_1 = h > 0$ and $\Xi_2 = 0$ to approximate a point on $\mathcal{M}_{\partial D}$ corresponding to the level set $W = w_0$. Based on the approximation (4.27), select $h > 0$ so that $w_0 = \frac{1}{2}h^2/U(y^*)$:

$$h = \sqrt{2w_0 U(y^*)}.$$

Now from (4.26) we calculate

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = hJ\mathbf{b}(y^*)$$

and from (4.25)

$$[P_1, P_2] = \frac{h}{U(y^*)|\mathbf{b}|^2} \mathbf{b}^T J.$$

Using these increments from $y^* \in \partial D$, $p = 0$ we obtain approximate coordinate values of the desired the point on $\mathcal{M}_{\partial D}$:

$$(4.29) \quad x_0 = y^* + hJ\mathbf{b}(y^*), \quad p_0 = \frac{h}{U(y^*)|\mathbf{b}|^2} \mathbf{b}^T J.$$

Finally, suppose we have a set of desired W -levels: $w_0 < w_1 < \dots < w_n$. We use w_0 and each of the approximate x_0, p_0 from (4.29) initial values to integrate (4.2) and (4.11) backwards in time, stopping at the times that $w(t_i) = w_i$ and recording the point $x(t_i)$ as a (possible) point of the level set $\{W = w_i\}$. These are then plotted to produce the figures of the previous section.

§5: PROOF OF THE SUFFICIENCY THEOREM

The goal of this final section is to prove Theorem 1. The following intermediate result will occupy most of our effort.

Theorem 2. *The following are all equivalent:*

(1) *For any $\delta > 0$ there exists $0 < w_0 < \delta$ so that V is constant over the W level set*

$$\{x \in D : W(x) = w_0\}.$$

(2) *V is smooth in \bar{D} .*

(3) *W is smooth in \bar{D} .*

(4) *$V(x) + W(x)$ is constant in \bar{D} .*

These equivalents provide a convenient link from Theorem 1 to the study of the cycling phenomenon in [2].

Proof (Theorem 1). Suppose as hypothesized in Theorem 1 that the level sets of V are not coincident with the level sets of W . Then (4) of Theorem 2 fails and hence so does (1). That means that for all sufficiently small $0 < w_0$, V is *not* constant over the level set

$$(5.1) \quad \{x \in D : W(x) = w_0\}.$$

We refer now to Section 4 of [2]. The discussion there concerned $\partial G = \{\rho(x) = \rho_0\}$ where $\rho(x) = \sqrt{W(x)}$ and ρ_0 is sufficiently small but otherwise arbitrary. Hence by taking $\rho_0 = \sqrt{w_0}$ sufficiently small, ∂G is identified with the level set in (5.1). The next to last paragraph of Section 4 of [2] explains why nonconvergent cycling must occur as a consequence of the non-constancy of V over ∂G .

We note the following corollary to Theorem 2.

Corollary. *If any of the conditions (1) – (4) of Theorem 2 are true then the manifolds \mathcal{M}_0 and $\mathcal{M}_{\partial D}$ coincide in phase space.*

This can be derived from condition (4) without much trouble, but it will come out directly in our proof of Theorem 2. We believe that $\mathcal{M}_0 = \mathcal{M}_{\partial D}$ is actually equivalent to the conditions of the theorem, but we have not proved it. We also conjecture that the coincidence of any one pair of (nonempty) level sets

$$\{W = c_W\} = \{V = c_V\}$$

is sufficient to imply the conditions of the theorem. Since Theorem 2 is adequate for our purposes as it stands we have not pursued these refinements.

We also comment that if the conditions (1) – (4) of Theorem 2 hold, then one can argue that each \mathcal{M}_0 bicharacteristic is V -minimizing along its full trajectory, i.e. to $x(t)$ for each t , and likewise are W -minimizing from each $x(t)$. This means that the set of $x(t_c)$ that we compute in finding the levels sets (either V or W) contain no extraneous points. I.e. there will be no fins! Hence the presence of fins means that (1) of Theorem 2 fails which, as we have seen, implies nonconvergent cycling of μ^ϵ .

We turn now to the proof.

Proof (Theorem 2). We will concentrate on the implications (1) \Rightarrow (2) \Rightarrow (4) \Rightarrow (1). Once that is done, then (2) \Rightarrow (2)&(4) from which (3) obviously follows. The argument for (3) \Rightarrow (4) is analogous to that of (2) \Rightarrow (4), as we will comment below.

Preliminaries There are constructions and notation which we want to develop before coming to grips with the assertions of the theorem.

Consider the ellipse

$$E = \{x : x^T S^{-1} x = \epsilon\}.$$

For small $\epsilon > 0$, E will be contained in the neighborhood N_0 where V is smooth. We claim that if $\epsilon > 0$ is sufficiently small then E parameterizes the phase trajectories of \mathcal{M}_0 ; i.e. there is a one-to-one correspondence between the $x_0 \in E$ and those phase trajectories $x(\cdot), p(\cdot)$ which satisfy

$$(5.2) \quad x(t_0) = x_0 \in E \quad \text{and} \quad p(t_0) = dV(x_0) \quad \text{for some } t_0.$$

We know that any phase trajectory satisfying (5.2) for some $x_0 \in E$ is on \mathcal{M}_0 . We need to show that each phase trajectory on \mathcal{M}_0 satisfies (5.2) for exactly one $x_0 \in E$.

Consider the function $\psi(x) = x^T S^{-1} x$. We know from (4.6) that any bicharacteristic on \mathcal{M}_0 has

$$(5.3) \quad p(t) = dV(x(t)),$$

at least until the first time τ_0 that $x(t)$ leaves N_0 . For all such $t < \tau_0$

$$(5.4) \quad \frac{d}{dt} \psi(x) = \langle 2x^T S^{-1}, \mathbf{b}(x) + a(x) dV^T(x) \rangle.$$

Now we know from (4.9) that

$$dV(x) = x^T S^{-1} + o(|x|) \quad \text{as } |x| \sim 0.$$

Using this and

$$b(x) = Bx + o(|x|) \quad \text{and} \quad a(x) = A + O(|x|)$$

we obtain

$$\begin{aligned} \frac{d}{dt} \psi(x) &= 2 \langle x^T S^{-1}, Bx + AS^{-1}x \rangle + o(|x|^2) \\ &= x^T S^{-1} AS^{-1} x + o(|x|^2). \end{aligned}$$

(The last equality is by virtue of (4.8).) The quadratic form occurring here is positive definite, so there exists $\epsilon_0 > 0$ so that $0 < \psi(x) \leq \epsilon_0$ implies both that $x \in N_0$ and that the right side of (5.4) is positive. Hence for any bicharacteristic on \mathcal{M}_0 both (5.3) and (5.4) hold, with (5.4) strictly positive, until after the first time $\psi(x(t)) \geq \epsilon_0$. Since $\psi(x(t)) \rightarrow 0$ as $t \rightarrow -\infty$, there must exist t_0 as in (5.2), provided $0 < \epsilon < \epsilon_0$. Moreover for any such t_0 , $\psi(x(t))$ is strictly increasing on $(-\infty, t_0]$. This implies that t_0 is unique.

The correspondence (5.2) defines a map $\pi_0 : N_0 \setminus \{0\} \rightarrow E$, where $x_0 = \pi_0(x)$ is the point on E satisfying (5.2) for the phase trajectory passing through the point x , $p = dV(x)$ on \mathcal{M}_0 . π_0 can be shown to be smooth, using the implicit function theorem.

We want to establish a similar parameterization of $\mathcal{M}_{\partial D}$ by a level set

$$C = \{x \in D : W(x) = w_0\}.$$

Take any $w_0 < \delta_1$, where δ_1 is as in the definition of $N_{\partial D}$. Suppose $x(\cdot), p(\cdot)$ is a bicharacteristic on $\mathcal{M}_{\partial D}$. From (4.10) the set of t for which

$$x(t) \in N_{\partial D}, \quad \text{and} \quad p(t) = -dW(x(t))$$

is the interval $\tau_1 < t$, where τ_1 is the smallest time at which $W(x(\tau_1)) \leq \delta_1$. For t in this interval $W(x(t))$ is strictly decreasing:

$$(5.5) \quad \frac{d}{dt}W(x) = \frac{1}{2}\langle p, a(x)p^T \rangle < 0.$$

Hence there exists a unique $x_1 = x(t_1)$ such that $W(x_1) = w_0$, that is

$$(5.6) \quad x(t_1) \in C \quad \text{and} \quad p(t_1) = -dW(x(t_1)) \quad \text{for some } t_1.$$

Conversely we know that if (5.6) holds for some $x_1 \in C$ then the phase path is on $\mathcal{M}_{\partial D}$. This shows that there is a one-to-one correspondence between $x_1 \in C$ and the phase trajectories on $\mathcal{M}_{\partial D}$, described by (5.6). Moreover the map $\pi_1 : N_{\partial D} \setminus \partial D \rightarrow C$ which takes x to $x_1 = \pi_1(x)$ satisfying (5.6) for the phase trajectory through x , $p = -dW(x)$ is smooth.

(1) implies (2) We assume that V is constant over C with w_0 sufficiently small to satisfy the preceding. Note this constant must be $V|_C = v_{\partial D} - w_0$. Indeed since there exist paths ϕ from C to ∂D with $S_{0T}(\phi)$ arbitrarily close to w_0 we must have $v_{\partial D} \leq V|_C + w_0$. On the other hand if $v_{\partial D} < V|_C + w_0$ then there would exist a ϕ from 0 to ∂D with $S_{0T}(\phi) < V|_C + w_0$. ϕ must pass through C at some $t \in (0, T)$. Since $S_{0t}(\phi) \geq V(\phi(t)) = V|_C$ we would have

$$\begin{aligned} V|_C + w_0 &> S_{0T}(\phi) \\ &= S_{0t}(\phi) + S_{tT}(\phi) \\ &\geq V|_C + S_{tT}(\phi), \end{aligned}$$

which implies $S_{tT}(\phi) < w_0$. This is impossible since as a path from $\phi(t) \in C$ to $\phi(T) \in \partial D$ we must have $S_{tT}(\phi) \geq w_0$.

Consider any $x_1 \in C$. Since $V(x_1) < v_{\partial D}$ there exists a V -minimizing bicharacteristic $x(\cdot), p(\cdot)$ to $x_1 = x(t_1)$. As a V -minimizer it must belong to the \mathcal{M}_0 family. We claim that it must also satisfy (5.6), which will show that the V -minimizer to x_1 is unique and belongs to the $\mathcal{M}_{\partial D}$ family as well. Let t_0 be as in (5.5) and let $x_0 = x(t_0)$. Then $x(\cdot)$ must achieve the minimum of

$$\int_{t_0}^{t_1} L(\phi, \dot{\phi}) dt$$

over all absolutely continuous ϕ on $[t_0, t_1]$ with $\phi(t_0) = x_0$ and $\phi(t_1) \in C$. Indeed if there were such a ϕ with a smaller value of $\int_{t_0}^{t_1} L$ than $x(\cdot)$, then by concatenating it with $x(\cdot)$ on $(-\infty, t_0]$ we would get a path from 0 to a point on C with a smaller value of V than $V(x_1)$. This is not possible since V is assumed constant over C . The transversality necessary condition for $x(\cdot)$ to solve this minimization problem implies that $p(t_1) = L_v(x(t_1), \dot{x}(t_1))$ is normal to C , i.e.

$$p(t_1) = c \cdot dW(x_1) \quad \text{for some } c \neq 0.$$

But we also know that both $H(x(t_1), p(t_1)) = 0$ and $H(x_1, -dW(x_1)) = 0$ hold. Since

$$\begin{aligned} 0 &= H(x, c \cdot dW(x)) \\ &= c^2 \langle dW(x), a(x)dW^T(x) \rangle - c \langle dW(x), \mathbf{b}(x) \rangle, \end{aligned}$$

there is at most one nonzero solution c . We conclude that $c = -1$ and so $p(t_1) = -dW(x(t_1))$. Hence (5.6) is indeed satisfied.

What we have shown is that for each $x_1 \in C$ there is a unique $x_0 \in E$ such the phase paths satisfying (5.2) and (5.6) coincide. Moreover this phase path is the unique V -minimizer to x_1 . We denote the map $x_0 \mapsto x_1$ so defined by $\Psi : C \rightarrow E$: $x_0 = \Psi(x_1)$. What we have said so far implies that $\mathcal{M}_{\partial D} \subseteq \mathcal{M}_0$. We intend to show that Ψ is surjective, which will mean that $\mathcal{M}_{\partial D} = \mathcal{M}_0$ (establishing the corollary stated above).

We claim that Ψ is continuous, and is an open map (i.e. it maps open subsets of C to open subsets of E .) Consider $x_1 \in C$ and $x_0 = \Psi(x_1) \in E$ with $x_0 = x(t_0)$, $x_1 = x(t_1)$ along a common bicharacteristic satisfying (5.2) and (5.6). Let $T = t_1 - t_0$. Observe that $\Psi(x) = \pi_0 \circ h_{-T}(x, -dW(x))$, at least for $x \in C$ sufficiently close to x_1 . This is because both sides produce a point on the same phase trajectory satisfying (5.2). By uniqueness they must agree. This shows that Ψ is smooth. Likewise $\tilde{\Psi} = \pi_1 \circ h_T(x, dV(x))$ defines a smooth function from a neighborhood of x_0 in E to C . Moreover $\tilde{\Psi} \circ \Psi(x) = x$ for all $x \in C$ sufficiently close to x_1 , because both sides are on the same phase trajectory and satisfy (5.6) and hence must agree. It follows from this that Ψ has nonvanishing Jacobian at $x_1 \in E$. (This Jacobian can be considered with respect to any convenient coordinate systems defined in neighborhoods of x_0 on E and x_1 on C .) Since $x_1 \in E$ was arbitrary, standard open mapping results now apply to tell us that Ψ is indeed an open mapping.

Since C is compact and Ψ is continuous, $\Psi(C) \subseteq E$ is closed. Since Ψ is open, and C is an open subset of itself, $\Psi(C)$ is also open in E . But the ellipse E is connected, so we conclude that $E = \Psi(C)$. This completes our demonstration that $\mathcal{M}_0 = \mathcal{M}_{\partial D}$, with the identification provided by Ψ via (5.2) and (5.6).

We are now in position to establish 2. Consider any $y \in D$. We can choose w_0 in the definition of C above so that $0 < w_0 < W(y)$. It follows that $V(y) \leq V|_C < v_{\partial D}$, so there exists a V -minimizing bicharacteristic $x(\cdot), p(\cdot)$ to $x(s) = y$. As a V -minimizer this must be a phase path from the \mathcal{M}_0 family. But since $\mathcal{M}_0 = \mathcal{M}_{\partial D}$ it also belongs to the $\mathcal{M}_{\partial D}$ family, and is the V -minimizer to some $x(t_1) = x_1 \in C$. Since $W(y) = W(x(s)) > w_0 = W(x(t_1))$ we must have $s < t_1$. Indeed, (5.6) implies $W(x(t)) \leq W(x(t_1))$ for all $t_1 \leq t$. Since $x(\cdot)$ is a V -minimizer to $x(t_1)$, V is smooth in a neighborhood of each $x(t)$ with $t < t_1$. In particular V is smooth in a neighborhood of $y = x(s)$. For y sufficiently near ∂D we know that $dV(y) = p(s) = -dW(y)$, since the V -minimizer to y and the W -minimizer from y are the same. Hence the smoothness of W up to and on ∂D implies the same for V . This completes the proof of 2.

(2) implies (4) We know $V \leq v_{\partial D}$, with equality on ∂D . We also know from [4] that

$$(5.7) \quad H(x, dV(x)) = 0$$

in $\Omega_0 = \{V < v_{\partial D}\}$. By continuity (5.7) extends to the closure $\bar{\Omega}_0$. Any point in $D \setminus \bar{\Omega}_0$ is interior to the set of x with $V(x) = v_{\partial D}$, and so has $dV(x) = 0$, for which (5.7) is also satisfied. Hence (5.7) holds in all of D .

We claim that $V(x) < v_{\partial D}$ for all interior points $x \in D$. Otherwise V would have an interior maximum, and so $dV(x_0) = 0$ at an interior point $x_0 \in D$. We will show that this is not possible. Now (5.7) implies, by the usual method of characteristics, that the solution $x(\cdot)$ of

$$\dot{x} = H_p(x, dV(x)); \quad x(0) = x_0$$

together with $p(\cdot)$ defined by

$$p(t) = dV(x(t))$$

is a solution of the Hamiltonian system (4.2), with initial conditions $x(0) = x_0$ and $p(0) = dV(x_0) = 0$. On the other hand $p(t) \equiv 0$ and the solution of (1.6) with $x(0) = x_0$ also solve (4.2) with the same initial conditions. Hence both solutions must coincide:

$$p(t) = dV(x(t)) \equiv 0,$$

and $x(t) \rightarrow 0$, because of our hypotheses on (1.6). But this would imply V is constant along $x(t)$ so that $0 = V(0) = V(x_0) = v_{\partial D} > 0$, a contradiction. Hence it must be that $V(x) < v_{\partial D}$ at all interior points of D , as claimed.

The function

$$\psi(x) = v_{\partial D} - V(x)$$

is a smooth solution of

$$(5.8) \quad H(x, -d\psi(x)) = 0$$

in \bar{D} which is 0 on ∂D and positive in D . The following “verification argument” will show that $\psi = W$. Consider any absolutely continuous $\phi : [0, T] \rightarrow \bar{D}$ with $\phi(0) = x_0$ and $\phi(T) \in \partial D$. Using (4.1) with $p = -d\psi(\phi)$ we find

$$L(\phi, \dot{\phi}) \geq \langle -d\psi, \dot{\phi} \rangle - H(\phi, -d\psi(\phi)) = -\frac{d}{dt}\psi(\phi).$$

Therefore

$$\int_0^T L(\phi, \dot{\phi}) \geq \psi(\phi(0)) - \psi(\phi(T)) = \psi(x_0),$$

showing that $W(x_0) \geq \psi(x_0)$. If we use the solution $x(\cdot)$ of

$$\dot{x} = H_p(x, -d\psi(x)), \quad x(0) = x_0$$

in place of $\phi(\cdot)$ above then equality holds when we invoke (4.1):

$$\frac{d}{dt}\psi(x) = -L(x, \dot{x}).$$

Using ψ as a Lyapunov function it follows that $x(t) \rightarrow \partial D$ and $\psi(x(t)) \rightarrow 0$ as $t \rightarrow \infty$. Taking $T \rightarrow \infty$ in

$$\int_0^T L(x, \dot{x}) = \psi(x_0) - \psi(x(T)).$$

we conclude that $W(x_0) \leq \psi(x_0)$. Thus $W(\cdot) \equiv \psi(\cdot) \equiv v_{\partial D} - V(\cdot)$, which is to say

$$V(\cdot) + W(\cdot) \equiv v_{\partial D} \quad \text{in } \bar{D}.$$

We comment that the proof of (3) \Rightarrow (4) is analogous: $\psi(x) = W(0) - W(x)$ is a smooth solution of $H(x, d\psi(x)) = 0$ which is nonnegative in D and 0 at the origin. (Lemma 1 of [RP] is also applicable.)

(4) implies (1) This is trivial; (4) implies that V is constant over a given set if and only if W is.

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