Numerical Analysis in Hamiltonian Dynamics

Chapter 1

The Problem

Consider a C^2-function $H : \mathbb{R}^{2n} \to \mathbb{R}$. The ordinary differential equations

$$\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i}(q,p)\,, \\ -\dot{p}_i &= \frac{\partial H}{\partial q_i}(q,p)\,, \end{aligned} \tag{1.1}$$

with $1 \leq i \leq n$, describe the evolution of many conservative systems in mechanics and are called Hamilton's equations. Here n is the number of degrees of freedom, $q = (q_1, \ldots, q_n) \in \mathbb{R}^n$ are the position and $p = (p_1, \ldots, p_n) \in \mathbb{R}^n$ are the momentum coordinates. The function H represents the energy of the system and is called the Hamiltonian. We deduce that H is constant along any solution of (1.1)

$$\frac{d}{dt}\left[H(q(t), p(t))\right] = 0\,,$$

i.e. H is an integral of motion. We will distinguish between solutions and orbits of (1.1): if $x(t)$ is a solution of (1.1) then $y(t) \equiv x(t+s)$, $s > 0$, obtained by time translation is a different solution but the same orbit. The Hamiltonian system (1.1) can be written more concisely with $z = (q,p) \in \mathbb{R}^{2n}$ as

$$\dot{z} = J_{2n} \nabla H(z)\,, \tag{1.2}$$

where $J_{2n} = \begin{pmatrix} 0 & Id_n \\ -Id_n & 0 \end{pmatrix} \in \mathcal{L}\left(\mathbb{R}^{2n} \times \mathbb{R}^{2n}\right)$ is the standard symplectic structure in $\mathbb{R}^{2n}$ and ∇H denotes the Euclidean gradient of H.

The existence of non-constant periodic orbits of (1.2) is a basic question of interest in the study of Hamiltonian systems. For any given $h > 0$, assume that the energy surface $S = \{x \in \mathbb{R}^{2n} | H(x) = h\}$ is regular, i.e. $\nabla H(x) \neq 0$ for all $x \in S$. Then the existence of periodic solutions on S of the Hamiltonian system (1.2) only depends on the geometry of S and is independent of the properties of the chosen H, see Hofer–Zehnder [14] § 1.5. For a convex H, a given energy level $h > 0$, and under some assumptions for the energy surface $S = H^{-1}(h)$, Ekeland and Lasry [11] show the existence of at least n distinct periodic orbits of the Hamiltonian flow with energy level h. Under different assumptions on H Ambrosetti and Mancini [3] give another proof of the statement by Ekeland and Lasry [11] and moreover, they proof a generalization. The method in the proof by Ambrosetti and Mancini is used by Mathlouthi [16] to find periodic solutions of a Hamiltonian system numerically, based on different assumptions than assumed below. Under the assumption that not the energy level h but the period is prescribed, the authors Rabinowitz [18], Clarke and Ekeland [5] and Ekeland [6] proof the existence of a non-constant periodic orbit under various assumptions on H.

We will determine periodic solutions of (1.2) via a numerical algorithm which is described in Chapter 2. This algorithm will give periodic solutions with the smallest action and can also be used to compute the symplectic capacity of open convex sets in phase space.

We consider a Hamiltonian $H : \mathbb{R}^{2n} \to \mathbb{R}$, $H \in C^2(\mathbb{R}^{2n} \setminus \{0\}, \mathbb{R})$, $H(0) = 0$, satisfying the assumptions (H) below:

H1. H is strictly convex

$$H(s\,x + (1-s)\,y) < s\,H(x) + (1-s)\,H(y)$$

for all $x, y \in \mathbb{R}^{2n}$, $s \in (0,1)$.

H2. H is positively homogeneous of degree two, i.e.

$$H(tx) = t^2 H(x),$$

for all $x \in \mathbb{R}^{2n}$ and $t > 0$.

H3. H has quadratic growth, i.e. there exist constants $c_1, c_2 > 0$ such that

$$c_1 \|x\|^2 \leq H(x) \leq c_2 \|x\|^2$$

for all $x \in \mathbb{R}^{2n}$.

We remark that the Hamiltonian system (1.2) with such a Hamiltonian H has at least n distinct periodic orbits on a given energy surface, see Ekeland–Lasry [11]. Moreover, note that via parametrization a periodic orbit of (1.2) with energy level h can be obtained from a periodic orbit of (1.2) with a different energy level h_1. Hence, in order to find periodic orbits of (1.2) on a prescribed energy surface, it is sufficient to look for periodic orbits of (1.2) with arbitrary energy levels.

The solutions of Hamilton's equations (1.2) are related to a functional, involving the Legendre transform $G : \mathbb{R}^{2n} \to \mathbb{R}$ of H, defined by

$$G(y) = \sup_{x \in \mathbb{R}^{2n}} \{\langle y, x \rangle_{\mathbb{R}^{2n}} - H(x)\}.$$

Since H is assumed to be strictly convex and of quadratic growth, we have

$$G(y) = \langle y, x \rangle_{\mathbb{R}^{2n}} - H(x) \tag{1.3}$$

with $x = \nabla H^{-1}(y)$ for all $y \in \mathbb{R}^{2n}$, see e.g. Amann [1] p. 45. G is a strictly convex C^2-function with $\nabla G(x) = \nabla H^{-1}(x)$ for all $x \in \mathbb{R}^{2n}$, and positively homogeneous of degree two. There exist constants $d_1, d_2 > 0$ with $d_1 \parallel x \parallel^2 \leq G(x) \leq d_2 \parallel x \parallel^2$, i.e. G has quadratic growth, the minimum of G lies in the origin and $G(0) = 0$.

Lemma 1 *$E = \{\dot{u} \in L^2([0,1], \mathbb{R}^{2n}) | \int_0^1 \dot{u}\, dt = 0\}$ is closed in $L^2([0,1], \mathbb{R}^{2n})$, hence a Hilbert space.*

Proof: Let $\{\dot{u}_n\}$ be a sequence in E, converging to $\dot{u}$ in L^2. Then

$$\left| \int_0^1 \dot{u}\, dt \right| = \left| \int_0^1 (\dot{u} - \dot{u}_n)\, dt \right| \leq \parallel \dot{u} - \dot{u}_n \parallel_{L^1} \leq \parallel \dot{u} - \dot{u}_n \parallel_{L^2}.$$

Because of $\lim_{n \to \infty} \parallel \dot{u} - \dot{u}_n \parallel_{L^2} = 0$ we deduce $\left| \int_0^1 \dot{u}\, dt \right| = 0$ and hence $\int_0^1 \dot{u}\, dt = 0$. □

We define the functional

$$F : E \longrightarrow \mathbb{R},\ F(\dot u) = \int_0^1 G\left(-J_{2n}\, \dot u(t)\right) dt\,. \tag{1.4}$$

Theorem 1 *If a function $\dot u \in E$ is a solution of the minimization problem*

$$F(\dot u) \quad = \quad \int_0^1 G\left(-J_{2n}\, \dot u\right) dt \quad \longrightarrow min\,!$$

with the constraint

$$\int_0^1 \langle -J_{2n}\, \dot u, u\rangle_{\mathbb{R}^{2n}}\, dt - 1 = 0\,, \tag{1.5}$$

then the function

$$v\,(t) := 2\sqrt{\lambda} \int_0^{\frac{t}{2\lambda}} \dot u(s)\, ds + \frac{c}{\sqrt{\lambda}} \tag{1.6}$$

with a function $\dot u \in L^2\left([0,1], \mathbb{R}^{2n}\right)$, a constant c in (1.9) *and $\lambda = F(\dot u)$ is a (2λ)-periodic solution of the Hamiltonian system* (1.2) *on the energy surface $S = \{H \equiv 1\}$.*

Proof: The derivative of $\int_0^1 \langle -J_{2n}\, \dot u, \int_0^t \dot u(s)\, ds\rangle\, dt$ in direction of a function $\dot h \in L^2\left([0,1], \mathbb{R}^{2n}\right)$ is $2\int_0^1 \langle -J_{2n}\, \dot h, \int_0^t \dot u(s)\, ds\rangle\, dt$ and the derivative of $\int_0^1 G\left(-J_{2n}\, \dot u\right) dt$ in direction of $\dot h$ is $\int_0^1 \langle J_{2n}\, \nabla G\left(-J_{2n}\, \dot u\right), \dot h\rangle\, dt$. For a solution $\dot u$ of the minimization problem (1.5) we have

$$0 = \int_0^1 \langle \nabla G\left(-J_{2n} \dot u\right), -J_{2n} \dot h\rangle\, dt - \lambda \cdot 2 \int_0^1 \langle -J_{2n} \dot h, \int_0^t \dot u(s)\, ds\rangle\, dt \tag{1.7}$$

$$= \int_0^1 \langle \nabla G\left(-J_{2n} \dot u\right) - 2\lambda \int_0^t \dot u(s)\, ds, -J_{2n} \dot h\rangle\, dt \tag{1.8}$$

for all $\dot h \in E$, where λ denotes the Lagrangian multiplier. Considering all $\dot h \in E$, (1.8) is equivalent to

$$\nabla G\left(-J_{2n} \dot u\right) - 2\lambda \int_0^t \dot u(s)\, ds = c, \tag{1.9}$$

or respectively,

$$-J_{2n} \dot u = \nabla H\left(2\lambda \int_0^t \dot u(s)\, ds + c\right), \tag{1.10}$$

with a constant $c \in \mathbb{R}^{2n}$. Because of $\dot w\,(t) = \dot u\left(\frac{t}{2\lambda}\right)$ and (1.10), the function

$$w\,(t) := 2\lambda \int_0^{\frac{t}{2\lambda}} \dot u(s)\, ds + c$$

is a (2λ)-periodic solution of the Hamiltonian system (1.2). We compute $H(w(t)) \equiv \lambda$ and hence

$$v\,(t) := 2\sqrt{\lambda} \int_0^{\frac{t}{2\lambda}} \dot u(s)\, ds + \frac{c}{\sqrt{\lambda}}$$

is a (2λ)-periodic solution of (1.2) on $S = \{H \equiv 1\}$. The period of v equals twice the Lagrange multiplier λ. We deduce from (1.7), choosing a solution $\dot u$ of (1.5) for $\dot h$,

$$\lambda = \int_0^1 G\left(-J_{2n} \dot u\right) dt = F(\dot u)\,. \tag{1.11}$$

□

Considering the minimization problem (1.5) is reasonable since a solution exists.

Theorem 2 *Suppose the Hamiltonian $H : \mathbb{R}^{2n} \to \mathbb{R}$ satisfies the assumptions* (H), *then there exists a solution of the minimization problem* (1.5).

Proof: Consider

$$M := \{\dot u \in E \mid \int_0^1 \langle -J_{2n}\, \dot u, u\rangle\, dt = 1\}\,.$$

Denote by $(\dot u_k)$ a minimizing sequence of F on M. Since G has quadratic growth, we have

$$F(\dot u) = \int_0^1 G\left(-J_{2n}\, \dot u\right) dt \geq \int_0^1 c\, \| -J_{2n}\, \dot u \|^2\ dt = c\, \| \dot u \|_{L^2}^2\,,$$

and thus $(\dot{u}_k)$ is bounded. Since L^2 is a Hilbert space, hence reflexive, $(\dot{u}_k)$ has a subsequence, also denoted by $(\dot{u}_k)$, that converges weakly to $\dot{u} \in L^2$, i.e. $\dot{u}_k \rightharpoonup \dot{u} \in L^2$. We have to show $\dot{u} \in M$. Denote by $\dot{u}_k^{(i)}(t)$ the ith coordinate of $\dot{u}_k(t)$. With $\dot{u}_k^{(i)} \rightharpoonup \dot{u}^{(i)}$ for $1 \le i \le 2n$ we see $\lim_{k\to\infty} \int_0^1 \dot{u}_k^{(i)}(t)dt = 0$ for $1 \le i \le 2n$, i.e. $\dot{u}$ satisfies the second constraint. We have $u_k \rightharpoonup u$ in $H^{1,2}([0,1],\mathbb{R}^{2n})$. Since the embedding $H^{1,2} \hookrightarrow L^2$ is compact, we deduce from the weak convergence $u_k \rightharpoonup u$ in $H^{1,2}$ that (u_k) in L^2 has a subsequence, again denoted by (u_k), that converges to u in L^2, i.e. $u_k \to u$ in L^2. The operator

$$-J_{2n}\frac{d}{dt} : \begin{cases} H^{1,2} & \longrightarrow & L^2 \\ u & \longmapsto & -J_{2n}\frac{d}{dt}u \end{cases}$$

is continuous, hence maps weakly convergent sequences to weakly convergent sequences, and we have $-J_{2n}\frac{d}{dt}u_k \rightharpoonup -J_{2n}\frac{d}{dt}u$, i.e. $-J_{2n}\dot{u}_k \rightharpoonup -J_{2n}\dot{u}$ in L^2. We deduce $\lim_{k\to\infty}\int_0^1 \langle -J_{2n}\dot{u}_k, u_k\rangle\, dt = \int_0^1 \langle -J_{2n}\dot{u}, u\rangle\, dt = 1$ and hence $\dot{u} \in M$.

It remains to show $F(\dot{u}) \le \lim_{k\to\infty} F(\dot{u}_k)$. There is a constant $c \in \mathbb{R}$ with $\lim_{k\to\infty} F(\dot{u}_k) < c$ and without loss of generality $F(\dot{u}_k) < c$ for all $k \in \mathbb{N}\setminus\{0\}$. Denote by C the convex hull of $\{\dot{u}_k | \, k \in \mathbb{N}\setminus\{0\}\}$. Then $\dot{u}$ lies in the weak closure of C which equals the strong closure of C since C is convex. Thus, there exists a sequence $(\dot{v}_n)_{n\in\mathbb{N}}$ in C that is strongly converging to $\dot{u}$, i.e. $(\dot{v}_n)$ has the properties

a) $\dot{v}_n \to \dot{u}$,

b) any $\dot{v}_n$ is a convex combination of finitely many $\dot{u}_k$, i.e.

$$\dot{v}_n = \sum_{k=1}^{\infty} \alpha_{nk}\,\dot{u}_k \text{ with } \sum_{k=1}^{\infty}\alpha_{nk} = 1\,, \quad \alpha_{nk} \ge 0$$

and for any n there are only finitely many $\alpha_{nk} \ne 0$.

Hence,

$$\begin{aligned} F(\dot{u}) &= \lim_{n\to\infty} F(\dot{v}_n) \\ &\le \lim_{n\to\infty}\sum_{k=1}^{\infty}\alpha_{nk}\,F(\dot{u}_k) \\ &< \sum_{k=1}^{\infty}\alpha_{nk}\cdot c = c\,. \end{aligned}$$

Since $\lim F(\dot{u}_k) < c$ arbitrarily, we have $F(\dot{u}) \le \lim F(\dot{u}_k)$, i.e. we have $F(\dot{u}) = \inf_M F$. □

The numerical algorithm that will be introduced in Chapter 2 gives a solution of the minimization problem (1.5). We now give a more general version of Theorem 1 where both statements are equivalent, since we consider critical points and not only minima of F.

For arbitrary $T \in \mathbb{R}$ consider

$$K_{2T} := \{z \in H^{1,2}([0,2T],\mathbb{R}^{2n}) | \int_0^{2T} \dot{z}\, dt = 0\}.$$

Our aim is to find solutions of

$$\{\dot{z} = J\nabla H(z), z \in K_{2T}, T \in \mathbb{R} \text{ arbitrary }, H(z) \equiv 1\}. \tag{1.12}$$

Theorem 3 *Consider $\dot{u}_0 \in E$. The following two statements are equivalent:*

(i) *$\dot{u}_0$ is a critical point of F on* $M = \{\dot{u} \in E | \int_0^1 \langle -J_{2n}\dot{u}, u\rangle_{\mathbb{R}^{2n}}\, dt - 1 = 0\}$.

(ii) *For a constant $c \in \mathbb{R}^{2n}$ and $T \in \mathbb{R}$ the function* $z(t) = 2\sqrt{T}\,u_0\left(\frac{t}{2T}\right) + c$, $z \in K_{2T}$, *is a $2T$-periodic solution of* (1.12).

Proof: We assume (i). Then

$$0 = \langle F'(\dot{u}_0), \dot{h}\rangle_{L^2} - \lambda\langle f'(\dot{u}_0), \dot{h}\rangle_{L^2} \tag{1.13}$$

for all $\dot{h} \in E$ and where λ is the Lagrangian multiplier. In Theorem 1 we deduced from (1.13) that the function

$$v\,(t) := 2\sqrt{\lambda}\int_0^{\frac{t}{2\lambda}} \dot{u}_0(s)\, ds + \frac{c}{\sqrt{\lambda}}$$

is a (2λ)-periodic solution of the Hamiltonian system (1.2) on $\{H \equiv 1\}$ with $\lambda = F(\dot{u}_0)$ and $c = \nabla G\,(-J_{2n}\dot{u}_0) - 2\,\lambda\int_0^t \dot{u}_0(s)\, ds$.

Vice versa, we assume (ii). With a change of parametrization we write z as

$$z(t) = 2\sqrt{T}\,u\Big(\frac{t}{2T}\Big) + \frac{\tilde{c}}{\sqrt{T}}$$

for an $u \in K_1$ and $\tilde{c} \in \mathbb{R}^{2n}$.

We obtain the derivative

$$\dot{z}(t) = \frac{1}{\sqrt{T}} \dot{u}\left(\frac{t}{2T}\right) = J\,\nabla H(z) = J\,\nabla H\left(2\sqrt{T} u\left(\frac{t}{2T}\right) + \frac{\tilde{c}}{\sqrt{T}}\right). \tag{1.14}$$

Since H is positive homogeneous of degree two we have

$$\frac{1}{2}\int_0^{2T} \langle -J\dot{z}, z\rangle\, dt = \frac{1}{2}\int_0^{2T} \langle \nabla H(z), z\rangle\, dt = \int_0^{2T} H(z)\, dt = 2T.$$

Together with

$$\int_0^{2T} \langle -J\dot{z}, z\rangle\, dt = \int_0^{2T} \langle -J\frac{1}{\sqrt{T}}\,\dot{u}\left(\frac{t}{2T}\right), 2\sqrt{T}\,u\left(\frac{t}{2T}\right)\rangle\, dt$$
$$= 4T\int_0^1 \langle -J\dot{u}(s), u(s)\rangle\, ds$$

we deduce

$$\int_0^1 \langle -J\dot{u}, u\rangle\, ds = 1,$$

hence $\dot{u} \in M$.

With $s := \frac{t}{2T}$, from (1.14) we obtain

$$\dot{u}(s) = J\,\nabla H\left(2Tu(s) + \tilde{c}\right),$$

equivalently,

$$\nabla G(-J\dot{u}(s)) - 2Tu(s) = \tilde{c}.$$

Hence we have

$$\int_0^1 \langle \nabla G(-J\dot{u}(s)) - 2Tu(s), -J\dot{h}(s)\rangle\, ds = 0$$

for all $\dot{h} \in E$, or equivalently

$$\langle F'(\dot{u}) - Tf'(\dot{u}), \dot{h}\rangle_E = 0$$

for all $\dot{h} \in E$ which is equivalent to

$$F'(\dot{u}) - Tf'(\dot{u}) = 0 \text{ in } E^*.$$

From $\dot{v} \in T_{\dot{u}}M \Leftrightarrow \langle f'(\dot{u}), \dot{v}\rangle = 0$ we deduce

$$\langle F'(\dot{u}), \dot{v}\rangle_E = T\langle f'(\dot{u}), \dot{v}\rangle_E = 0$$

for all $\dot{v} \in T_{\dot{u}}M$. □

Chapter 2

The Numerical Algorithm

In order to solve the minimization problem (1.5) by a numerical algorithm it has to be discretized. The discretization of (1.5) is described and discussed in Section 2.1. The interval $[0,1]$ is divided in m equidistant subintervals and we consider the space of functions $\tilde{u} : [0,1] \to \mathbb{R}^{2n}$, constant on each subinterval. Each of these so-called step functions is uniquely assigned via the values on the subintervals to a vector in $(\mathbb{R}^{2n})^m$. With this identification the discretized problem is proposed. The existence of a solution of the discretized problem is shown.

2.1 The Discretized Problem

Dividing the interval $[0,1]$ into m equidistant subintervals we consider functions $\tilde{u} : [0,1] \to \mathbb{R}^{2n}$ that are constant on each subinterval $[t_j, t_{j+1}[$ with $t_j := \frac{j}{m}$, $0 \le j \le m-1$, with $\tilde{u}(1)$ chosen as $\tilde{u}(1) = \tilde{u}(t_{m-1})$. We call $\tilde{u}$ a step function on $[0,1]$ with respect to the m subintervals $[t_j, t_{j+1}[$, $0 \le j \le m-1$. Denote by $T = T\left(t_0, .., t_m, [0,1], \mathbb{R}^{2n}\right)$ the vector space of these step functions. We uniquely assign to each function $\tilde{u} \in T$ a vector $x = (x_0, .., x_{m-1}) = (x_0^{(1)}, .., x_0^{(2n)}, .., x_{m-1}^{(1)}, .., x_{m-1}^{(2n)}) \in$

$(\mathbb{R}^{2n})^m$:

$$x_j := \tilde{u}(t) \quad \text{for} \quad t \in [t_j, t_{j+1}[\,,\ 0 \le j \le m-1\,. \tag{2.1}$$

Denoting the restriction of the functional F in (1.4) to the space T also by F, we have

$$F(x) = \frac{1}{m} \sum_{j=0}^{m-1} G(-J_{2n}\, x_j)\,. \tag{2.2}$$

With the identification (2.1) we have

$$\int_0^t \tilde{u}(s)\, ds = \frac{1}{m} \sum_{j=0}^{k-1} x_j + (t - t_k)\, x_k$$

for $t_k \le t \le t_{k+1}$, and hence

$$\begin{aligned}
\int_0^1 \langle -J_{2n}\, \tilde{u}(t), \int_0^t \tilde{u}(s)\, ds\rangle\, dt &= \sum_{k=0}^{m-1} \int_{t_k}^{t_{k+1}} \langle -J_{2n}\, \tilde{u}(t), \int_0^t \tilde{u}(s)\, ds\rangle\, dt \\
&= \sum_{k=0}^{m-1} \langle -J_{2n}\, x_k, \frac{1}{m^2} \sum_{j=0}^{k-1} x_j + \frac{1}{2m^2}\, x_k\rangle \\
&= \frac{1}{m^2} \sum_{k=1}^{m-1} \sum_{j=0}^{k-1} \langle -J_{2n}\, x_k, x_j\rangle \qquad (2.3) \\
&= \frac{1}{m^2}\, x^T A_{2n}\, x\,, \qquad (2.4)
\end{aligned}$$

with

$$A_{2n} := \begin{pmatrix} 0_{2n} & -J_{2n} & \dots & -J_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & -J_{2n} \\ 0_{2n} & \dots & \dots & 0_{2n} \end{pmatrix} \in \mathcal{L}\left((\mathbb{R}^{2n})^m \times (\mathbb{R}^{2n})^m\right). \tag{2.5}$$

We remark that in the computer program the term (2.3) is used, since the vector-matrix-vector-multiplication (2.4) leads to a higher computational and stack effort. But for describing and discussing the numerical algorithm using (2.4) is more reasonable.

With (2.1) the constraint $\int_0^1 \tilde{u}\, dt = 0$ of the minimization problem (1.2) is written as

$$\sum_{j=0}^{m-1} x_j = 0\,. \tag{2.6}$$

Condition (2.6) consists of $2n$ conditions, $g_i(x) = 0$ for $1 \le i \le 2n$, where

$$g_i : \left\{ \begin{array}{ccc} (\mathbb{R}^{2n})^m & \longrightarrow & \mathbb{R} \\ x & \longmapsto & \sum_{j=0}^{m-1} x_j^{(i)} \end{array} \right. \tag{2.7}$$

for $1 \le i \le 2n$. Let $\{e_i^{(2n)} \in \mathbb{R}^{2n} | \, 1 \le i \le 2n\}$ be the set of canonical unit vectors in $\mathbb{R}^{2n}$. With $a^{(i)} := (e_i^{(2n)}, .., e_i^{(2n)})^T \in (\mathbb{R}^{2n})^m$ we have

$$g_i(x) = \langle a^{(i)}, x\rangle\,, \tag{2.8}$$

for $1 \le i \le 2n$, $x \in (\mathbb{R}^{2n})^m$. We formulate the discretized minimization problem:

$$F(x) = \frac{1}{m} \sum_{j=0}^{m-1} G(-J_{2n}\, x_j)\,,\ x \in (\mathbb{R}^{2n})^m, \quad \longrightarrow min!$$

with the two constraints

$$\begin{aligned}
&1) \quad f(x) \equiv \frac{1}{m^2}\, x^T A_{2n}\, x - 1 = 0 \\
&2) \quad g_i(x) = \langle a^{(i)}, x\rangle = 0 \quad \text{for } 1 \le i \le 2n\,.
\end{aligned} \tag{2.9}$$

Consider

$$M_m := \{x \in (\mathbb{R}^{2n})^m | \, f(x) = g_1(x) = .. = g_{2n}(x) = 0\}\,. \tag{2.10}$$

M_m is a differentiable $(2nm - 2n - 1)$-dimensional manifold. We assume $m \ge 3$, otherwise in (2.9) both conditions cannot be satisfied. The derivatives of f and F in $x \in (\mathbb{R}^{2n})^m$ are

$$\nabla f(x) = \frac{1}{m^2}\, (A_{2n} + A_{2n}^T)\, x \tag{2.11}$$

and

$$\nabla F(x) = \frac{1}{m}\, \left(J_{2n} \nabla G\,(-J_{2n} x_0), .., J_{2n} \nabla G\,(-J_{2n} x_{m-1})\right). \tag{2.12}$$

Before discussing the numerical algorithm for solving the discretized minimization problem (2.9) we proof the existence of a solution.

Theorem 4 *Suppose the Hamiltonian H satisfies condition* (H), *then there exists a solution of problem* (2.9).

PROOF: Consider a minimizing sequence $(y_l)_{l\in\mathbb{N}}$ of F on M_m. Since G has quadratic growth we have

$$F(x) \geq \frac{c}{m}\sum_{j=0}^{m-1} \| x_j \|^2_{\mathbb{R}^{2n}} = \frac{c}{m} \| x \|^2_{\left(\mathbb{R}^{2n}\right)^m},$$

with a constant $c > 0$. Hence (y_l) is bounded and has a subsequence converging to $y \in (\mathbb{R}^{2n})^m$, which lies on M_m since the constraints in problem (2.9) are continuous. □

Before describing and discussing the numerical algorithm in detail we summarize the steps in a clear way.

2.2 Formulation of the Algorithm

I. Calculation of a solution of problem (2.9)

Denote by $x_0 \in M_m$ the starting point of the iteration and $x_k \in M_m$, $k \in \mathbb{N}$, is the k th iteration point.

1. Compute

$$\begin{aligned}
a_k &= \nabla f(x_k) = \frac{1}{m^2}\,(A_{2n} + A_{2n}^T)\,x_k\,,\\
y_k &= -\nabla F(x_k)\,,\\
a_{kH} &= a_k - \frac{1}{m}\left(\langle a^{(1)}, a_k\rangle\, a^{(1)} + .. + \langle a^{(2n)}, a_k\rangle\, a^{(2n)}\right),\\
\hat{y}_k &= y_k - \frac{\langle a_{kH}, y_k\rangle}{\langle a_{kH}, a_{kH}\rangle}\, a_{kH} - \frac{1}{m}\Big(\langle a^{(1)}, y_k\rangle a^{(1)} + .. + \langle a^{(2n)}, y_k\rangle a^{(2n)}\Big).
\end{aligned}$$

2. If $\hat{y}_k = 0$, then the iteration ends and $x_{min} := x_k$ solves the minimization problem (2.9).

3. If $\hat{y}_k \neq 0$, then compute

$$\begin{aligned}
\lambda_{max} &= \sqrt{\frac{3}{4}}\,\frac{m}{\sqrt{|\,\hat{y}_k^T A_{2n}\,\hat{y}_k\,|}}\,,\\
h_k(\lambda_{max}) &= \langle \hat{y}_k, -\nabla F\,(x_k + \lambda_{max}\,\hat{y}_k)\rangle\,,\\
h_k(0) &= \langle \hat{y}_k, \hat{y}_k\rangle\,.
\end{aligned}$$

If $h_k(\lambda_{max}) \geq 0$ then $\lambda_0 := \lambda_{max}$, else

$$\lambda_0 := \lambda_{max}\,\frac{h_k(0)}{h_k(0) - h_k(\lambda_{max})}\,.$$

Compute:

$$\begin{aligned}
c_{\lambda_0} &= \frac{1}{m^2}\,\lambda_0^2\,\hat{y}_k^T\,A_{2n}\,\hat{y}_k + 1\,,\\
x_{\lambda_0} &= x_k + \lambda_0\,\hat{y}_k\,,\\
x_{M_{\lambda_0}} &= \frac{1}{\sqrt{c_{\lambda_0}}}\,x_{\lambda_0}\,,\\
\delta_1 &= F(x_k) - F(x_{\lambda_0})\,,\\
\delta_2 &= F(x_k) - F(x_{M_{\lambda_0}})\,.
\end{aligned}$$

If $\delta_2 \leq \frac{1}{4}\,\delta_1$ then repeat

$$\lambda_0 := \frac{\lambda_0}{2} \quad \text{and compute } c_{\lambda_0}, x_{\lambda_0}, x_{M_{\lambda_0}}, \delta_1 \text{ and } \delta_2 \text{ as above}$$

until $\delta_2 > \frac{1}{4}\,\delta_1$. If $\delta_2 > \frac{1}{4}\,\delta_1$ then the iteration step ends and $x_{k+1} := x_{M_{\lambda_0}}$ becomes the next iteration point.

II. Calculation of a solution of the Hamiltonian system (1.2)

The above calculated solution of problem (2.9) is denoted by x_{min}. Compute

$$\lambda = \frac{1}{m}\sum_{j=0}^{m-1} G\,(-J_{2n}x_{min_j})\,. \tag{2.13}$$

The value of a (2λ)-periodic solution v of the Hamiltonian system (1.2) in $\hat{t}_k := 2\,\lambda\,\frac{k}{m}$, $0 \leq k \leq m-1$, is

$$v(\hat{t}_k) = \frac{2\sqrt{\lambda}}{m}\sum_{j=0}^{k-1} x_{min_j} + \frac{1}{\sqrt{\lambda}\,m}\sum_{j=0}^{m-1} \nabla G\,(-J_{2n}\,x_{min_j})$$

$$-\frac{2\sqrt{\lambda}}{m^2}\sum_{i=1}^{m-1}\sum_{j=0}^{i-1}x_{min_j}\,. \tag{2.14}$$

2.3 Derivation of the Algorithm

In the following the algorithm will be discussed in detail. Denote the starting point of the iteration by $x_0 \in M_m$ and the iteration point in the kth iteration step by $x_k \in M_m$. The proposed algorithm determines a solution of the minimization problem via a modified method of projected gradients. In the kth step, starting from $x_k \in M_m$ the gradient $-\nabla F(x_k)$ is projected with respect to the linearized first constraint and the second constraint of (2.9). The vectors a_k and y_k are denoted as in the algorithm above. Define

$$H := \{z \in (\mathbb{R}^{2n})^m \,|\, \langle a^{(1)}, z\rangle = .. = \langle a^{(2n)}, z\rangle = 0\}\,, \tag{2.15}$$

$$H_k := \{z \in H \,|\, \langle a_k, z\rangle = 0\}\,. \tag{2.16}$$

Because of $x_k \in M_m$, the vectors a_k, $a^{(1)}, \ldots, a^{(2n)}$ are linearly independent. Hence, H_k is a $(2nm-2n-1)$-dimensional and H a $(2nm-2n)$-dimensional subspace of $(\mathbb{R}^{2n})^m$. Because of $\langle a_k, x_k\rangle \neq 0$ we have $x_k \notin H_k$. Denote the orthogonal projection of a vector $z \in (\mathbb{R}^{2n})^m$ on H_k with $\hat{z}$. In the kth iteration step the vector y_k is projected onto H_k and if $\hat{y}_k \in H_k$ is not the null vector we determine the minimum of F on the line $x_k + \lambda\,\hat{y}_k$, $\lambda \geq 0$; as will be explained later, not the entire line $\{x_k + \lambda\,\hat{y}_k,\ \lambda \geq 0\}$ can be considered for the minimum search. Since $x_k \in H$ we have

$$x_k + H_k = \{z \in H \,|\, \langle a_k, z - x_k\rangle = 0\}\,.$$

As a first step we consider the orthogonal projection of a vector $z \in (\mathbb{R}^{2n})^m$ on H, denoted by $z_H \in H$:

$$\begin{aligned} z_H &= z - \frac{\langle a^{(1)}, z\rangle}{\langle a^{(1)}, a^{(1)}\rangle}\,a^{(1)} - .. - \frac{\langle a^{(2n)}, z\rangle}{\langle a^{(2n)}, a^{(2n)}\rangle}\,a^{(2n)} \\ &= z - \frac{1}{m}\left(\langle a^{(1)}, z\rangle\, a^{(1)} + .. + \langle a^{(2n)}, z\rangle\, a^{(2n)}\right), \end{aligned} \tag{2.17}$$

since $a^{(1)}, .., a^{(2n)}$ are pairwise orthogonal. The vector a_k is not orthogonal to $a^{(1)}, .., a^{(2n)}$. To derive a simple form for the projection onto H_k,

we first project a_k onto H via (2.17) and obtain a_{kH}. Then projecting y_k onto H_k with respect to $a^{(1)}, .., a^{(2n)}$ and a_{kH} we obtain

$$\hat{y}_k = y_k - \frac{\langle a_{kH}, y_k\rangle}{\langle a_{kH}, a_{kH}\rangle}\,a_{kH} - \frac{1}{m}\left(\langle a^{(1)}, y_k\rangle\, a^{(1)} + .. + \langle a^{(2n)}, y_k\rangle\, a^{(2n)}\right). \tag{2.18}$$

The vector x_k is a solution of (2.9) iff

$$\hat{y}_k = 0. \tag{2.19}$$

This criterion of optimality is a reformulation of the "local" Kuhn–Tucker conditions, see Künzi–Krelle [15] p. 63, in the case where the constraints consist only of equations. Intuitively, condition (2.19) means that starting in x_k, in no direction on $x_k + H_k$ an improvement is possible; the iteration ends and $x_{min} := x_k$ is a solution of (2.9).

If $\hat{y}_k \neq 0$, the next iteration step is carried out. The vectors $\{x_k + \lambda\,\hat{y}_k,\ \lambda \geq 0\}$ satisfy the constraint $g_i(x) = 0$, $1 \leq i \leq 2n$ of problem (2.9). But because of $x_k \in M_m$ and $\langle a_k, \hat{y}_k\rangle = 0$ there exists no $\lambda > 0$ such that $x_k + \lambda\,\hat{y}_k$ satisfies the first constraint of problem (2.9). Suppose the minimum of F among the vectors $\{x_k + \lambda\,\hat{y}_k,\ \lambda \geq 0\}$ is in $x_k + \lambda_0\,\hat{y}_k$, $\lambda_0 \neq 0$. This point has to be led back to M_m. We have

$$\frac{1}{m^2}\,(x_k + \lambda\,\hat{y}_k)^T A_{2n}\,(x_k + \lambda\,\hat{y}_k) = \frac{1}{m^2}\,\lambda^2\,\hat{y}_k^T A_{2n}\,\hat{y}_k + 1\,. \tag{2.20}$$

If

$$0 < \frac{1}{m^2}\,\lambda_0^2\,\hat{y}_k^T A_{2n}\,\hat{y}_k + 1 =: c_{\lambda_0}\,, \tag{2.21}$$

then we have $\frac{1}{\sqrt{c_{\lambda_0}}}\,(x_k + \lambda_0\,\hat{y}_k) \in M_m$. In the case $\hat{y}_k^T A_{2n}\,\hat{y}_k < 0$ condition (2.21) is satisfied if we assume the upper bound for λ

$$\lambda_{max} := \frac{m}{\sqrt{|\,\hat{y}_k^T A_{2n}\,\hat{y}_k\,|}}\,. \tag{2.22}$$

We remark that in the numerical algorithm in condition (2.21) we consider as lower bound $\frac{1}{4}$ instead of 0. As upper bound for λ we obtain $\sqrt{\frac{3}{4}}\lambda_{max}$, again denoted by λ_{max}. Since no point $x_k + \lambda\,\hat{y}_k$, $\lambda > 0$, satisfies the first constraint of problem (2.9) and because of (2.20), the case $\hat{y}_k^T A_{2n}\,\hat{y}_k = 0$ is not possible. In the case $\hat{y}_k^T A_{2n}\,\hat{y}_k > 0$ there is no upper bound for $\lambda > 0$, but in order to avoid a too small scaling factor $\frac{1}{\sqrt{c_{\lambda_0}}}$, we also choose λ_{max} as upper bound here.

We want to find

$$\min_{0 \le \lambda \le \lambda_{max}} F(x_k + \lambda\, \hat{y}_k)\,.$$

The projection of the negative gradient of F in $x_k + \lambda\, \hat{y}_k$, $0 \le \lambda \le \lambda_{max}$, onto $\{x_k + \lambda\, \hat{y}_k,\ 0 \le \lambda \le \lambda_{max}\}$ is

$$\frac{1}{\|\, \hat{y}_k \,\|^2} \langle \hat{y}_k, -\nabla F\,(x_k + \lambda\, \hat{y}_k)\rangle\, \hat{y}_k\,.$$

Consider the function

$$h_k : \begin{cases} [0, \lambda_{max}] & \longrightarrow \mathbb{R} \\ \lambda & \longmapsto \langle \hat{y}_k, -\nabla F\,(x_k + \lambda\, \hat{y}_k)\rangle\,. \end{cases} \tag{2.23}$$

Lemma 2 *h_k is strictly decreasing.*

PROOF: Since F is strictly convex, we have for any λ_1, $\lambda_2 \in [0, \lambda_{max}]$

$$\begin{aligned} F(x_k + \lambda_2\, \hat{y}_k) - F(x_k + \lambda_1\, \hat{y}_k) &> (\lambda_2 - \lambda_1)\, \langle \hat{y}_k, \nabla F(x_k + \lambda_1\, \hat{y}_k)\rangle \\ &= (\lambda_1 - \lambda_2)\, h_k(\lambda_1)\,. \end{aligned} \tag{2.24}$$

Hence for any $\lambda_1 < \lambda_2$

$$h_k(\lambda_1) > \frac{F(x_k + \lambda_2\, \hat{y}_k) - F(x_k + \lambda_1\, \hat{y}_k)}{\lambda_1 - \lambda_2} > h_k(\lambda_2)\,.$$

□

We have $h_k(0) = \|\, \hat{y}_k \,\|^2 > 0$. Two cases are to distinguish depending on $h_k(\lambda_{max})$.

a) If $h_k(\lambda_{max}) \ge 0$, then $h_k(\lambda) \ge 0$ for $0 \le \lambda \le \lambda_{max}$. Because of (2.24), on the line between x_k and $x_k + \lambda_{max}\, \hat{y}_k$ F is strictly decreasing and hence the smallest value is attained in $x_k + \lambda_{max}\, \hat{y}_k$.

b) If $h_k(\lambda_{max}) < 0$, there exists a unique λ' with $h_k(\lambda') = 0$. From (2.24) we deduce that the smallest value of F on the line between x_k and $x_k + \lambda_{max}\, \hat{y}_k$ is attained in $x_k + \lambda'\, \hat{y}_k$. We approximate λ' via linear interpolation:

$$\lambda' := \lambda_{max} \frac{h_k(0)}{h_k(0) - h_k(\lambda_{max})}\,. \tag{2.25}$$

Note that for quadratic G the function h_k is linear and (2.25) is exact.

Denote the obtained minimum of F on the line between x_k and $x_k + \lambda_{max}\, \hat{y}_k$ by $x_{\lambda_0} := x_k + \lambda_0\, \hat{y}_k$. With c_{λ_0} in (2.21) we have $\frac{1}{\sqrt{c_{\lambda_0}}}\, x_{\lambda_0} =: x_{M_{\lambda_0}} \in M_m$. The improvement achieved in x_{λ_0} is $\delta_1 := F(x_k) - F(x_{\lambda_0})$. If this improvement is partially transferred to $x_{M_{\lambda_0}}$, more precisely if

$$\delta_2 := F(x_k) - F(x_{M_{\lambda_0}}) > \frac{1}{4}\, \delta_1\,, \tag{2.26}$$

then the iteration step ends and $x_{k+1} := x_{M_{\lambda_0}}$ is the new iteration point. Otherwise, we halve the line between x_k and x_{λ_0} and denoting $\frac{\lambda_0}{2}$ again by λ_0 we check (2.26). We halve and check iteratively until (2.26) is true and the iteration step ends with $x_{k+1} := x_{M_{\lambda_0}}$.

The entire iteration ends if the projected negative gradient $\hat{y}_k$ in x_k is the null vector, and $x_{min} := x_k$ solves problem (2.9).

We assign the computed solution x_{min} of (2.9) via (2.1) to a step function $\tilde{u}_{min}$. With (1.6), (1.9) and (1.11) we immediately obtain the formulae for v (2.14) and λ (2.13).

For the iteration method proposed in 2.2.I. above, we give a global theorem of convergence.

Theorem 5 *Denote by $(x_k)_{k\in\mathbb{N}}$ a sequence on M_m obtained by the iteration method in 2.2.I. Then $(x_k)_{k\in\mathbb{N}}$ has an accumulation point $\bar{x} \in M_m$ with $\hat{\bar{y}} = 0$, where $\bar{y} := -\nabla F(\bar{x})$.*

PROOF: For $c_0 := F(x_0)$ consider $N_{c_0} := \{x \in (\mathbb{R}^{2n})^m |\ F(x) \le c_0\}$. N_{c_0} is bounded, since

$$F(x) \ge \frac{c}{m} \sum_{j=0}^{m-1} \|\, x_j \,\|^2_{\mathbb{R}^{2n}} = \frac{c}{m}\ \|\, x \,\|^2_{(\mathbb{R}^{2n})^m}\,.$$

Because of $F(x_k) < F(x_{k-1})$ for all $k \in \mathbb{N}$, $(x_k)_{k\in\mathbb{N}} \subset N_{c_0}$. Hence, $(x_k)_{k\in\mathbb{N}} \subset M_m$ is bounded and has an accumulation point $\bar{x} \in M_m$, since M_m is closed.

It remains to show $\hat{\bar{y}} = 0$. Assume $\hat{\bar{y}} \ne 0$, and starting in $\bar{x}$ the next iteration step gives us a point x_s on the line between $\bar{x}$ and $\bar{x} + \lambda_{max}\hat{\bar{y}}$. Transferring x_s to M_m we get a point $x_{M_m} \in M_m$ with

$$F(\bar{x}) - F(x_{M_m}) > \frac{1}{4}\,(F(\bar{x}) - F(x_s)) =: c_1\,,$$

where $c_1 > 0$ since F is strictly convex. There exists a $\varepsilon_0 > 0$ with

$$F(\bar{x}) > c_1 + \frac{\varepsilon_0}{2} + F(x_{M_m}).$$

Since F is continuous there exist neighborhoods $U_{\bar{x}} \subset (\mathbb{R}^{2n})^m$ around $\bar{x}$ and $U_{x_{M_m}} \subset (\mathbb{R}^{2n})^m$ around x_{M_m} with

$$F(x_1) > c_1 + \frac{\varepsilon_0}{2} + F(x_2) \tag{2.27}$$

for all $x_1 \in U_{\bar{x}}$ and $x_2 \in U_{x_{M_m}}$. The projection of the negative gradient of F and F are continuous in x, hence there exists an $\varepsilon > 0$ with $B_\varepsilon(\bar{x}) \subset U_{\bar{x}}$, such that $|F(\bar{x}) - F(x_1)| < \varepsilon_0$ and $\hat{y}_1 \neq 0$ for all $x_1 \in B_\varepsilon(\bar{x})$ and $y_1 := -\nabla F(x_1)$. Moreover, there exists a neighborhood U_{x_s} around x_s with $\mid F(x_s) - F(x_{s_1}) \mid < \varepsilon_0$ for all $x_{s_1} \in U_{x_s}$ and such that via transferring to M_m all $x_{s_1} \in U_{x_s}$ are mapped into $U_{x_{M_m}}$. There exists an $\varepsilon' > 0$ with $B_{\varepsilon'}(\bar{x}) \subset B_\varepsilon(\bar{x})$ such that starting an iteration step from any $x_{\varepsilon'} \in B_{\varepsilon'}(\bar{x})$ we obtain a point $x_{\varepsilon'_s} \in U_{x_s}$ on the line $x_{\varepsilon'}$ to $x_{\varepsilon'} + \lambda_{max}\hat{y}_{\varepsilon'}$, with obvious notation. Transferring $x_{\varepsilon'_s}$ to M_m we get $x_{\varepsilon'_M} \in U_{x_{M_m}}$. For any $x_{\varepsilon'} \in B_{\varepsilon'}(\bar{x})$ and $x_{s_1} \in U_{x_s}$ we have

$$\begin{aligned} \mid F(x_{\varepsilon'}) - F(x_{s_1}) \mid &\leq \mid F(x_{\varepsilon'}) - F(\bar{x}) \mid + \mid F(\bar{x}) - F(x_s) \mid \\ &\quad + \mid F(x_s) - F(x_{s_1}) \mid \\ &< 2\varepsilon_0 + 4c_1 . \end{aligned} \tag{2.28}$$

From (2.27) we see

$$F(x_{\varepsilon'}) > c_1 + \frac{\varepsilon_0}{2} + F(x_{\varepsilon'_M}),$$

and hence with (2.28)

$$F(x_{\varepsilon'}) > \frac{1}{4}(F(x_{\varepsilon'}) - F(x_{\varepsilon'_s})) + F(x_{\varepsilon'_M}), \tag{2.29}$$

for all $x_{\varepsilon'} \in B_{\varepsilon'}(\bar{x})$. (2.29) means that starting the iteration step in any $x_{\varepsilon'} \in B_{\varepsilon'}(\bar{x})$, the next iteration point is $x_{\varepsilon'_M} \in U_{x_{M_m}}$. In $B_{\varepsilon'}(\bar{x})$ there are infinitely many points of the iteration sequence. From this sequence choose an $x_{k_0} \in B_{\varepsilon'}(\bar{x})$. For x_{k_0} (2.29) is satisfied. Because of (2.27) from x_{k_0+1} on no iteration point lies in $B_{\varepsilon'}(\bar{x})$ which is a contradiction. □

Chapter 3

Application of the Algorithm

3.1 Symplectic Capacities

The proposed numerical algorithm cannot only be used to approximate periodic orbits of a Hamiltonian system on a strictly convex bounded energy surface, but can also be used to calculate symplectic invariants of open convex sets in phase space. Ekeland and Hofer [9, 10] discovered these symplectic invariants, called symplectic capacities, for subsets of $\mathbb{R}^{2n}$ and Hofer and Zehnder [13] extended the concept of symplectic capacities to general symplectic manifolds.

Our aim is to approximate via the numerical algorithm symplectic capacities of several examples of strictly convex bounded and smooth energy surfaces. These examples will be investigated at the end of this section. But first, we recall some background material, following Hofer and Zehnder [14]. We give the definition of a symplectic vector space, symplectic manifolds and symplectic mappings. Then we see that the Hamiltonian flow is a symplectic map. The axioms of a symplectic capacity are given. Considering positive quadratic forms in $\mathbb{R}^{2n}$, it turns out that for subsets of $\mathbb{R}^{2n}$ the symplectic capacity extends a linear symplectic invariant for these forms to nonlinear symplectic mappings.

Then a special symplectic capacity c_0 is constructed by means of Hamiltonian systems. For a convex bounded and smooth domain C in $\mathbb{R}^{2n}$ it equals the minimal action of periodic solutions on ∂C.

In Section 3.2 we show that assuming we have a global minimum of (1.5) obtained by the proposed algorithm, the derived periodic solution on the energy surface has minimal action. Finally, in Section 3.3 we investigate four different strictly convex bounded and smooth domains in $\mathbb{R}^{2n}$ concerning the capacity c_0 and the minimal action of periodic solutions on the boundary. We will further consider these examples in Section 3.4.

Consider a finite dimensional real vector space V together with a non-degenerate antisymmetric bilinear form ω, i.e. for every $u \in V$, $u \neq 0$, there exists a $v \in V$ with $\omega(u,v) \neq 0$ and

$$\omega(u,v) = -\omega(v,u)$$

for all $u, v \in V$. (V,ω) is called a *symplectic vector space.*

As a special case we consider the symplectic vector space $(\mathbb{R}^{2n}, \omega_0)$ with

$$\omega_0(u,v) \equiv \langle J\,u, v\rangle$$

for all $u, v \in \mathbb{R}^{2n}$, where $\langle .,. \rangle$ denotes the Euclidean scalar product in $\mathbb{R}^{2n}$ and

$$J = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}.$$

The pair $(\mathbb{R}^{2n}, \omega_0)$ is called the *standard-symplectic vector space.* With the coordinates $(x_1, .., x_n, y_1, .., y_n) \in \mathbb{R}^{2n}$ we write ω_0 as the 2-form

$$\omega_0 = \sum_{j=1}^{n} dy_j \wedge dx_j.$$

A linear map $A : V \mapsto V$ of (V, ω) is called *symplectic*, if

$$A^*\omega = \omega,$$

where $A^*\omega$ is defined by $A^*\omega(u,v) = \omega(Au, Av)$. $A^*\omega$ is called *pullback 2-form.* Hence, we have in $(\mathbb{R}^{2n}, \omega_0)$ that a matrix A is symplectic if and only if

$$\langle J\,Au, Av\rangle = \langle J\,u, v\rangle$$

for all $u, v \in \mathbb{R}^{2n}$, or equivalently,

$$A^T J A = J.$$

It can be deduced that $\det A = 1$, hence symplectic matrices in $\mathbb{R}^{2n}$ are volume preserving, see Hofer–Zehnder [14], p. 4f. Symplectic matrices are a group under matrix multiplication, denoted by $Sp(n)$.

We now consider nonlinear maps in $(\mathbb{R}^{2n}, \omega_0)$. A diffeomorphism φ in $\mathbb{R}^{2n}$ is called *symplectic* if

$$\varphi^*\omega_0 = \omega_0,$$

where for an arbitrary 2-form ω we have

$$(\varphi^*\omega)_x(a,b) = \omega_{\varphi(x)}(\varphi'(x)\,a, \varphi'(x)\,b),$$

with $x \in \mathbb{R}^{2n}$, $a, b \in T_x\mathbb{R}^{2n} = \mathbb{R}^{2n}$. We deduce that $\varphi'(x)$ is a symplectic matrix. Hence, symplectic diffeomorphisms are volume preserving. Because of

$$\omega_0 = \sum_{j=1}^{n} dy_j \wedge dx_j = d\lambda$$

with the 1-form

$$\lambda = \sum_{j=1}^{n} y_j\, dx_j,$$

ω_0 is exact. Thus, if φ is a symplectic diffeomorphism, we have $d(\lambda - \varphi^*\lambda) = d\lambda - \varphi^* d\lambda = \omega_0 - \varphi^*\omega_0 = 0$. That is, $\lambda - \varphi^*\lambda$ is a closed form and with Poincaré's lemma we find a function $F : \mathbb{R}^{2n} \mapsto \mathbb{R}$ with

$$\lambda - \varphi^*\lambda = dF.$$

Consider a oriented simply closed curve γ. Since the integral of an exact form over a closed curve vanishes we have

$$\int_\gamma \lambda = \int_\gamma \varphi^*\lambda = \int_{\varphi(\gamma)} \lambda.$$

We define the *action* $\mathcal{A}(\gamma)$ of a closed curve γ as

$$\mathcal{A}(\gamma) := \int_\gamma \lambda \in \mathbb{R}.$$

Hence we have

$$\mathcal{A}(\varphi(\gamma)) = \mathcal{A}(\gamma),$$

i.e., a symplectic diffeomorphism is not only volume preserving but also keeps the action invariant. Consider a parametrization of γ denoted by $x(t)$ with $0 \leq t \leq 1$, $x(0) = x(1)$. For the action we obtain

$$\begin{aligned}\mathcal{A}(\gamma) &= \frac{1}{2}\int_0^1 \langle -J\dot{x}, x\rangle\, dt \\ &= \frac{1}{2}\int_0^T \langle -J\dot{v}, v\rangle\, ds,\end{aligned}$$

with $v(s) \equiv x\left(\frac{s}{T}\right)$, $s \in [0, T]$.

In the same way as the gradient field ∇H of H with respect to the Euclidean scalar product is defined

$$dH(x)\, y = \langle \nabla H(x), y\rangle_{\mathbb{R}^{2n}},$$

we define the vector field X_H of H with respect to the symplectic form ω_0

$$\begin{aligned} dH(x)y &= \omega_0(-X_H(x), y) &(3.1)\\ &= \langle -J\, X_H(x), y\rangle_{\mathbb{R}^{2n}}. &(3.2)\end{aligned}$$

Hence, we have the following relationship between the so called Hamiltonian vector field X_H and the gradient field ∇H

$$X_H(x) = J\,\nabla H(x).$$

Consider $H : \mathbb{R}^{2n} \mapsto \mathbb{R}$ Hamiltonian function, X_H Hamiltonian vector field of H and $\tau : \mathbb{R}^{2n} \mapsto \mathbb{R}^{2n}$ symplectic diffeomorphism, i.e. $\tau^*\omega_0 = \omega_0$. Define $K = H \circ \tau$, X_K Hamiltonian vector field of K. Then we have the following transformation formula

$$X_K = (d\tau)^{-1} \cdot X_H \circ \tau. \qquad (3.3)$$

If τ is a linear symplectic (bijective) transformation we have

$$X_{H\circ\tau} = \tau^{-1} \cdot H \cdot \tau. \qquad (3.4)$$

Denote by φ^t the flow of the Hamiltonian vector field $J\,\nabla H$, i.e. we have

$$\begin{aligned}\frac{d}{dt}\varphi^t(x) &= J\,\nabla H\left(\varphi^t(x)\right) &(3.5)\\ \varphi^0(x) &= x, \quad x \in \mathbb{R}^{2n}. &(3.6)\end{aligned}$$

Then $x(t) = \varphi^t(x)$ solves the initial value problem with initial value x. It can be shown that every flow φ^t of $J\,\nabla H$ preserves the form ω_0

$$\left(\varphi^t\right)^* \omega_0 = \omega_0,$$

i.e., the Hamiltonian flow φ^t is a symplectic map.

Definition 1 *Consider two open subsets $U, V \subset \mathbb{R}^{2n}$. Then the map $\varphi : U \mapsto \mathbb{R}^{2n}$ with $\varphi^*\omega_0 = \omega_0$ and $\varphi(U) \subset V$ is called a* symplectic embedding.

Note that $\mathrm{vol}(U) \leq \mathrm{vol}(V)$ since a symplectic embedding is volume preserving.

Now we introduce a symplectic structure on an even dimensional manifold.

Definition 2 *A symplectic structure on an even dimensional manifold M is a 2-form ω on M with*

(i) $d\omega = 0$, i.e., ω is a closed form,

(ii) ω is nondegenerate.

A symplectic structure is nondegenerate if on every tangent space T_xM we have: $\omega_x(u, v) = 0$ for all $v \in T_xM \Rightarrow u = 0$. Such a pair (M, ω) is called a symplectic manifold.

We now give the axioms of a special class of symplectic invariants for symplectic manifolds of dimension $2n$ and possibly with boundary. These symplectic invariants are called symplectic capacities. They were discovered by Ekeland and Hofer [9, 10] for subsets of $\mathbb{R}^{2n}$ and were extended to general symplectic manifolds by Hofer and Zehnder [13].

Definition 3 *Consider the class of $2n$-dimensional symplectic manifolds (M, ω) possibly with boundary. A symplectic capacity is a map $(M, \omega) \mapsto c(M, \omega)$ with $c(M, \omega) \in \mathbb{R}^+ \cup \{\infty\}$, satisfying the following three properties:*

A1: *Monotonicity* $c(M,\omega) \leq c(N,\tau)$, *if there exists an embedding* $\varphi : (M,\omega) \mapsto (N,\tau)$.

A2: *Conformality* $c(M,\alpha\omega) = |\alpha|\, c(M,\omega)$, *for all* $\alpha \in \mathbb{R}, \alpha \neq 0$.

A3: *Nontriviality* $c(B(1),\omega_0) = \pi = c(Z(1),\omega_0)$, *where* $B(r) = \{(x,y) \in \mathbb{R}^{2n} | |x|^2 + |y|^2 < r^2\}$, $Z(r) = \{(x,y) \in \mathbb{R}^{2n} | x_1^2 + y_1^2 < r^2\}$, $r > 0$.

Remarks: 1. The symplectic capacity is not uniquely determined.

2. Consider a symplectic diffeomorphism $\varphi : (M,\omega) \mapsto (N,\tau)$ between two manifolds M and N. Applying **A1** to φ and to φ^{-1} we verify that the capacity is a symplectic invariant

$$c(M,\omega) = c(N,\tau).$$

In the following we consider subsets in the standard-symplectic space $(\mathbb{R}^{2n},\omega_0)$.

Lemma 3 *For* $U \subset (\mathbb{R}^{2n},\omega_0)$ *open and* $\lambda \in \mathbb{R}, \lambda \neq 0$ *we have*

$$c(\lambda U) = \lambda^2\, c(U).$$

PROOF: see Hofer–Zehnder [14], p. 52. □

We deduce

$$c\,(B(r)) = r^2 c\,(B(1)) = \pi\, r^2. \tag{3.7}$$

And analogously,

$$c\,(Z(r)) = \pi\, r^2. \tag{3.8}$$

If U is an open subset with

$$B(r) \subset U \subset Z(r),$$

for an $r > 0$, then with **A1** we see

$$\pi\, r^2 = c\,(B(r)) \leq c(U) \leq c\,(Z(r)) = \pi\, r^2,$$

hence

$$c(U) = \pi\, r^2.$$

Before we discuss more general subsets of $(\mathbb{R}^{2n},\omega_0)$, first we investigate ellipsoids. Consider a positive definite quadratic form q on $(\mathbb{R}^{2n},\omega_0)$, i.e.,

$$q(x) = \frac{1}{2}\langle Sx, x\rangle$$

for $S = S^T$ positive definite matrix, $x \in \mathbb{R}^{2n}$. We denote the set of positive definite quadratic forms q on $(\mathbb{R}^{2n},\omega_0)$ by $\mathcal{P}$. The $Sp(n)$-action on $\mathcal{P}$ is defined by

$$\mathcal{P} \times Sp(n) \to \mathcal{P} : [q,p] \mapsto q \circ \varphi.$$

We assign q to the open ellipsoid $E(q)$

$$E(q) = \{x \,|\, q\ (x) < 1\} \subset \mathbb{R}^{2n}.$$

For two positive definite quadratic forms q_1, q_2 we have

$$E(q_1) \subset E(q_2) \Leftrightarrow q_1 \geq q_2, \tag{3.9}$$

hence

$$E(q_1) = E(q_2) \Leftrightarrow q_1 = q_2. \tag{3.10}$$

Moreover,

$$\begin{aligned}\varphi^{-1}(E(q)) &= \{\varphi^{-1}(x) | q(x) < 1\} \\ &= \{y | q \circ \varphi(y) < 1\} \\ &= E(q \circ \varphi)\,. \end{aligned} \tag{3.11}$$

Theorem 6 *Consider the standard-symplectic vector space* $(\mathbb{R}^{2n},\omega_0)$. *Let* q *be a positive definite quadratic form,* $q(x) = \langle Sx, x\rangle$ *with* S *symmetric and positive definite,* $x \in \mathbb{R}^{2n}$. *Then there exists a linear symplectic map* φ *on* $(\mathbb{R}^{2n},\omega_0)$ *with*

$$q \circ \varphi(x) = \frac{1}{2}\sum_{j=1}^{n} \lambda_j (x_j^2 + x_{n+j}^2), \tag{3.12}$$

with $0 < \lambda_n \leq \lambda_{n-1} \leq \ldots \leq \lambda_1$. *The* λ_j *are uniquely determined by* q *and* ω_0, *since* $(\pm i\lambda_j)$, $1 \leq j \leq n$, *are eigenvalues of the linear Hamiltonian vector field* X_q

$$\omega_0(X_q(x), y) = -dq(x)y \tag{3.13}$$

for all $x, y \in \mathbb{R}^{2n}$, *i.e.* $X_q(x) = JSx$.

Because of (3.3), X_q and $X_{q\circ\tau}$ are similar to each other, hence they have the same eigenvalues. We assign a positive definite quadratic form q to a vector $\lambda = \lambda(q) = (\lambda_1, .., \lambda_n) \in \mathbb{R}^n$ with the values $\lambda_j \in \mathbb{R}^+ \setminus \{0\}$, $1 \le j \le n$, determined in Theorem 6. We obtain

$$\lambda(q \circ \tau) = \lambda(q) \tag{3.14}$$

for all symplectic linear maps τ and for all positive definite quadratic forms q.

With a change of notation $\lambda_j = \frac{2}{r_j^2}$, $1 \le j \le n$, we assign each q to a vector $r(q) = r = (r_1(q), ..., r_n(q)) \in \mathbb{R}^n$ with $0 < r_1(q) \le r_2(q) \le ... \le r_n(q)$. Analogously to (3.14) we deduce

Proposition 1

$$r(q) = r(q \circ \varphi)$$

for all $q \in \mathcal{P}$ and for all $\varphi \in Sp(n)$. Moreover, if

$$r(q_1) = r(q_2),$$

for $q_1, q_2 \in \mathcal{P}$, then there exists a $\varphi \in Sp(n)$ with $q_1 = q_2 \circ \varphi$.

Proposition 2 *Consider $q_1, q_2 \in \mathcal{P}$. Then*

$$q_1 \le q_2 \Rightarrow r_j(q_2) \le r_j(q_1) \tag{3.15}$$

for $1 \le j \le n$.

PROOF: see Hofer–Zehnder [14].

Because of (3.9), (3.10) and (3.11) to each open ellipsoids E we can assign the number $r(E)$

$$r(E) := r(q), \tag{3.16}$$

for $E = E(q)$. With Proposition 1 and (3.11) we deduce

Proposition 3 *Let E, F be open ellipsoids in $(\mathbb{R}^{2n}, \omega_0)$ and $\varphi \in Sp(n)$, then $r(\varphi(E)) = r(E)$. Vice versa, if $r(E) = r(F)$, then there exists a $\varphi \in Sp(n)$ with $\varphi(E) = F$.*

PROOF: see Hofer–Zehnder [14].

From (3.9) and Proposition 2 we deduce the monotonicity property

Proposition 4 *Let E, F be open ellipsoids in $(\mathbb{R}^{2n}, \omega_0)$. Then*

$$E \subset F \Rightarrow r_j(E) \le r_j(F) \tag{3.17}$$

for $1 \le j \le n$. Vice versa, if $r_j(E) \le r_j(F)$ for $1 \le j \le n$, then there exists $\varphi \in Sp(n)$ with $\varphi(E) \subset F$.

PROOF: see Hofer–Zehnder [14].

Altogether, we obtain with Proposition 3 and Proposition 4

Theorem 7 *Let E, F be open ellipsoids in $(\mathbb{R}^{2n}, \omega_0)$. There exists a $\varphi \in Sp(n)$ with $\varphi(E) \subset F$ if and only if $r_j(E) \le r_j(F)$ for all $1 \le j \le n$.*

PROOF: see Hofer–Zehnder [14].

With Theorem 7 we may assume that $B(r_1) \subset E \subset Z(r_1)$ with $r_1 = r_1(E)$ and we have

Proposition 5 *The capacity of an ellipsoid E in $(\mathbb{R}^{2n}, \omega_0)$ is*

$$c(E) = \pi r_1(E)^2 .$$

More general, consider now a convex bounded domain $C \subset \mathbb{R}^{2n}$ with smooth boundary δC. Let H be a function, $H : \mathbb{R}^{2n} \mapsto \mathbb{R}$, having δC as regular energy surface, i.e., $\delta C = S := \{x | H(x) = \tilde{c}\}$, $\tilde{c} \in \mathbb{R}$, and $dH(x) \neq 0$ on S.

Denote by $\mathcal{D}$ the set

$$\mathcal{D} := \{\gamma | \gamma \text{ is periodic solution of } \dot{z} = J\,\nabla H(z) \text{ on } S\}. \tag{3.18}$$

We assign to each element $\gamma \in \mathcal{D}$ its action $\mathcal{A}$. In the following we want to determine

$$\inf \{|\mathcal{A}(\gamma)|\,|\gamma \in \mathcal{D}\} . \tag{3.19}$$

For a domain C as above there exist $r, R \in \mathbb{R}^+ \setminus \{0\}$ and two symplectic embeddings φ_1, φ_2 such that

$$\varphi_1(B(r)) \subset C, \varphi_2(C) \subset Z(R).$$

With axiom **A1** (monotonicity) we deduce

$$c(B(r)) \leq c(C) \leq c(Z(R)) \tag{3.20}$$

for any arbitrary symplectic capacity c. With (3.7) and (3.8) we see, with (3.20), that

$$\pi r^2 \leq c(C) \leq \pi R^2. \tag{3.21}$$

In Hofer–Zehnder [14] the existence of a special capacity c_0 on symplectic manifolds is proved. Here we will restrict ourselves to subsets of the standard-symplectic vector space $(\mathbb{R}^{2n}, \omega_0)$. Consider $U \subset (\mathbb{R}^{2n}, \omega_0)$, $H : U \mapsto \mathbb{R}$ a smooth function. Denote by $\mathcal{H}(U, \omega_0)$ the set of all smooth functions H on U with

- $(P1)$ There exists a compact set $K \subset U$, depending on H, with $K \subset (U \setminus \partial U)$ and $H(U \setminus K) \equiv m(H) \in \mathbb{R}$.
- $(P2)$ There exists an open set $V \subset U$, depending on H with $H(V) \equiv 0$.
- $(P3)$ For all $x \in U$: $0 \leq H(x) \leq m(H)$.

A function $H \in \mathcal{H}(U, \omega_0)$ is called *admissible*, if all periodic solutions of $\dot{x} = X_H(x)$ on U are either constant or have a period $T > 1$. The set of admissible functions is denoted by $\mathcal{H}_a(U, \omega_0) \subset \mathcal{H}(U, \omega_0)$. We define

$$c_0(U, \omega_0) = \sup\{m(H) | \, H \in \mathcal{H}_a(U, \omega_0)\}. \tag{3.22}$$

If in the case $c_0(U, \omega_0) < \infty$ we have $m(H) > c_0(U, \omega_0)$ with a function $H \in \mathcal{H}(U, \omega_0)$, then the corresponding Hamiltonian vector field X_H has a nonconstant T-periodic solution with $0 < T \leq 1$. Moreover, $c_0(U, \omega_0)$ is the infimum over all real numbers with this property. For the proof that c_0 is a capacity we refer to Hofer–Zehnder [14].

Theorem 8 *Let $C \subset \mathbb{R}^{2n}$ be a convex bounded domain with smooth boundary ∂C. Let $H : \mathbb{R}^{2n} \mapsto \mathbb{R}$ be a function having $\partial C =: S$ as regular energy surface. With $\mathcal{D}$ in (3.18) there exists a $\gamma^* \in \mathcal{D}$ with*

$$c_0(C, \omega_0) = |\mathcal{A}(\gamma^*)| = \inf\{|\mathcal{A}(\gamma)| \, |\gamma \in \mathcal{D}\}. \tag{3.23}$$

With (3.21) we deduce

$$\pi r^2 \leq c_0(C, \omega_0) = |\mathcal{A}(\gamma^*)| \leq \pi R^2, \tag{3.24}$$

i.e., we found an upper and a lower bound for the smallest action on S.

3.2 Minimal Action

In the following we show that the proposed numerical algorithm yields a periodic solution on $S = \{H \equiv 1\}$ with minimal action.

The action of a $2T$-periodic solution $z(t)$ of (1.12) can be calculated

$$A(z) = \frac{1}{2} \int_0^{2T} \langle -J\dot{z}, z \rangle \, dt = \frac{1}{2} \int_0^{2T} \langle \nabla H(z), z \rangle \, dt = \int_0^{2T} H(z) \, dt = 2T, \tag{3.25}$$

i.e., in the case of a 2-homogeneous Hamiltonian function H the action of a periodic solution of a Hamiltonian system on the energy surface $\{H \equiv 1\}$ equals the period of the solution.

For the action of $v(t)$ in (1.6) we obtain

$$A(v) = \frac{1}{2} \int_0^{2\lambda} \langle -J\dot{v}, v \rangle \, dt = 2\lambda.$$

Theorem 9 *Let $\dot{u}_0$ be a solution of* (1.5). *Among all solutions of* (1.12) *the function $v(t) = 2\sqrt{\lambda} \int_0^{\frac{t}{2\lambda}} \dot{u}_0(s) \, ds + \frac{c}{\sqrt{\lambda}}$ with $c = \nabla G(-J_{2n}\dot{u}_0) - 2\lambda \int_0^t \dot{u}_0(s) \, ds$, $\lambda = F(\dot{u}_0)$ and $T = \lambda$ is a solution with minimal action.*

PROOF: Let $z(t)$ be a solution of (1.12). As in the proof $((i) \Rightarrow (ii))$ of Theorem 3 we write $z(t)$ as

$$z(t) = 2\sqrt{T} \, u\left(\frac{t}{2T}\right) + \frac{\tilde{c}}{\sqrt{T}} \tag{3.26}$$

with a constant $\tilde{c} \in \mathbb{R}^{2n}$ and a function $u \in K_1$. In the proof of Theorem 3 we deduced $\dot{u} \in M$ and moreover,

$$\begin{aligned} & F'(\dot{u}) - T\, f'(\dot{u}) = 0 \text{ in } E^* \\ \Leftrightarrow \quad & \langle F'(\dot{u}) - T\, f'(\dot{u}), \dot{h} \rangle = 0 \end{aligned}$$

for all $\dot{h} \in E$. Hence

$$\begin{aligned}
&\langle F'(\dot{u}) - T f'(\dot{u}), \dot{u}\rangle = 0 \\
\Leftrightarrow\ & \int_0^1 \langle \nabla G(-J\dot{u}), -J\dot{u}\rangle\, dt - 2T \int_0^1 \langle u, -J\dot{u}\rangle\, dt = 0 \\
\Leftrightarrow\ & 2\int_0^1 G(-J\dot{u})\, dt - 2T = 0 \\
\Leftrightarrow\ & T = F(\dot{u}).
\end{aligned}$$

If $\dot{u}_0$ is a solution of (1.5), then $F(\dot{u})$ is minimized, i.e.

$$\frac{1}{2}\, A(z) = T = F(\dot{u}) \geq F(\dot{u}_0) = \lambda = \frac{1}{2}\, A(v),$$

i.e., $v(t)$ is a solution of the Hamiltonian system with minimal action. We remark that in the case where the algorithm yields a local minimum and not a global minimum of the minimization problem (1.5) we obtain a periodic solution of the Hamiltonian system (1.2) with an action that is not the smallest possible one on the energy surface. In this context see also Subsection 3.4.1.

3.3 Examples

In each of the following four examples we consider a strictly convex bounded domain with smooth boundary and find upper and lower bounds for the minimal action on the boundary. Theses examples are also used in Section 3.4 for investigating the numerical algorithm.

Example 1 As a special example consider the strictly convex domain C_1

$$C_1 := \left\{x \in \mathbb{R}^4 |\, r_1^2 + 4r_2^2 - 2r_1^2 r_2^2 < 1 \text{ and } r_1^2 < 1, r_2^2 < \frac{1}{4}\right\}, \qquad (3.27)$$

with $r_1^2 := x_1^2 + x_3^2$ and $r_2^2 := x_2^2 + x_4^2$. Our aim is to obtain with (3.24) an upper and a lower bound for the smallest action on $S_1 = \partial C_1$.

Proposition 6 $B(\frac{1}{2}) = \{x \in \mathbb{R}^4 |\, r_1^2 + r_2^2 < \frac{1}{4}\} \subset C_1$.

PROOF: For $x \in B(\frac{1}{2})$ we have

$$r_1^2 + 4\,r_2^2 - 2\,r_1^2 r_2^2 \leq r_1^2 + 4\,r_2^2 < 1.$$

□

Proposition 7 *The linear map* $\varphi_0(x_1, x_2, x_3, x_4) = (x_2, x_1, x_4, x_3)$ *is symplectic.*

PROOF: For the matrix A assigned to φ_0 we have $A^T J A = J$. □

We transform the cylinder

$$Z\left(\frac{1}{2}\right) = \left\{x \in \mathbb{R}^4 |\, r_1^2 < \frac{1}{4}\right\}$$

with φ_0 to

$$\tilde{Z}\left(\frac{1}{2}\right) := \varphi_0\left(Z\left(\frac{1}{2}\right)\right) = \left\{x \in \mathbb{R}^4 |\, r_2^2 < \frac{1}{4}\right\}.$$

Since the capacity is invariant under symplectic transformations and since $C_1 \in \tilde{Z}\left(\frac{1}{2}\right)$ we deduce

$$c(C_1) \leq c\left(\tilde{Z}\left(\frac{1}{2}\right)\right) = c\left(Z\left(\frac{1}{2}\right)\right) = \frac{\pi}{4}. \qquad (3.28)$$

Hence,

$$c\left(B\left(\frac{1}{2}\right)\right) \leq c(C_1) \leq c\left(Z\left(\frac{1}{2}\right)\right)$$

or equivalently

$$\frac{\pi}{4} \leq c(C_1) \leq \frac{\pi}{4}$$

for all capacities c. Thus we have

$$c_0(C_1) = |\mathcal{A}(\gamma^*)| = \frac{\pi}{4}$$

with γ^* in Theorem 8, i.e. the minimal action on S_1 is $\frac{\pi}{4}$.

Example 2 Consider the strictly convex domain C_2

$$C_2 := \left\{x \in \mathbb{R}^4 |\, r_1^4 + 4\,r_2^4 < 1\right\}, \qquad (3.29)$$

with $r_1^2 := x_1^2 + x_3^2$ and $r_2^2 := x_2^2 + x_4^2$.

Proposition 8 $B(\frac{1}{\sqrt{2}}) = \{x \in \mathbb{R}^4 | r_1^2 + r_2^2 < \frac{1}{2}\} \subset C_2$.

PROOF: For $x \in B(\frac{1}{\sqrt{2}})$ we have

$$r_1^4 + 4\,r_2^4 \leq r_1^4 + 4\,r_1^2 r_2^2 + 4\,r_2^4 = (r_1^2 + 2\,r_2^2)^2 < 1.$$

□

Proposition 9 *With* φ_0 *as in* Proposition 7,

$$C_2 \subset \tilde{Z}\left(\frac{1}{\sqrt{2}}\right) := \varphi_0\left(Z\left(\frac{1}{\sqrt{2}}\right)\right) = \left\{x \in \mathbb{R}^4 | r_2^2 < \frac{1}{2}\right\}. \qquad (3.30)$$

PROOF: With $x \in C_2$ we have

$$r_1^4 + 4\,r_2^4 < 1 \Rightarrow 4\,r_2^4 < 1 \Rightarrow r_2^2 < \frac{1}{2}. \qquad (3.31)$$

□

As regards the capacity we obtain

$$\frac{\pi}{2} = c\left(B\left(\frac{1}{\sqrt{2}}\right)\right) \leq c(C_2) \leq c\left(\tilde{Z}\left(\frac{1}{\sqrt{2}}\right)\right) = \frac{\pi}{2},$$

i.e., $c(C_2) = \frac{\pi}{2}$ for all capacities c, especially for c_0. Hence, the minimal action on $S_2 = \partial C_2$ is $\frac{\pi}{2}$.

Example 3 Consider the strictly convex domain C_3

$$C_3 := \Big\{x \in \mathbb{R}^4 \,|\, \frac{1}{2}(x_1^2 + x_3^2) + x_2^2 + x_4^2 + \frac{1}{10}\Big[\sin(x_1 + x_2 + x_3 + x_4) + \cos(x_1 + x_2 + x_3 + x_4)\Big] < 1\Big\}.$$

Proposition 10 *Consider* $c_1 = \sqrt{1 - \frac{\sqrt{2}}{10}}$. *Then*

$$B(c_1) \subset C_3. \qquad (3.32)$$

PROOF: For $x \in B(c_1)$ we have

$$\begin{aligned} & \frac{1}{2}(x_1^2 + x_3^2) + x_2^2 + x_4^2 \\ & + \frac{1}{10}\Big[\sin(x_1 + x_2 + x_3 + x_4) + \cos(x_1 + x_2 + x_3 + x_4)\Big] \\ \leq\ & x_1^2 + x_3^2 + x_2^2 + x_4^2 + \frac{\sqrt{2}}{10} \\ <\ & c_1^2 + \frac{\sqrt{2}}{10} = 1\,. \end{aligned}$$

□

Proposition 11 *With the constant* $c_2 := \sqrt{1 + \frac{\sqrt{2}}{10}}$ *and* φ_0 *as in* Proposition 7, *we have that*

$$C_3 \subset \tilde{Z}(c_2) := \varphi_0(Z(c_2)) = \{x \in \mathbb{R}^4 \,|\, x_2^2 + x_4^2 < c_2^2\}. \qquad (3.33)$$

PROOF: For $x \in C_3$ we have

$$\begin{aligned} 1 >\ & \frac{1}{2}(x_1^2 + x_3^2) + x_2^2 + x_4^2 \\ & + \frac{1}{10}\Big[\sin(x_1 + x_2 + x_3 + x_4) + \cos(x_1 + x_2 + x_3 + x_4)\Big] \\ \geq\ & \frac{1}{2}(x_1^2 + x_3^2) + x_2^2 + x_4^2 - \frac{\sqrt{2}}{10} \\ \geq\ & x_2^2 + x_4^2 - \frac{\sqrt{2}}{10}, \end{aligned}$$

and hence

$$x_2^2 + x_4^2 < 1 + \frac{\sqrt{2}}{10} = c_2^2\,.$$

□

For the capacity of C_3 we obtain the bounds

$$\begin{gathered} \pi c_1^2 = c(B(c_1)) \leq c(C_3) \leq c(\tilde{Z}(c_2)) = \pi c_2^2 \\ 2.6973 \leq c(C_3) \leq 3.5859, \end{gathered} \qquad (3.34)$$

i.e., the minimal action on $S_3 = \partial C_3$ lies between 2.69 and 3.59.

Example 4 For the strictly convex domain

$$C_4 := \left\{x \in \mathbb{R}^4 \mid r_1^4 + r_2^4 < 1\right\}, \tag{3.35}$$

we have

$$B(1) \subset C_4 \subset Z(1), \tag{3.36}$$

and hence

$$c(C_4) = \pi, \tag{3.37}$$

for all capacities c, i.e. the minimal action on $S_4 = \partial C_4$ is π.

3.4 Evaluation of the Algorithm

We applied the numerical program to the four examples in Section 3.3. In the following we list and discuss the results. In each example a domain is given with a strictly convex boundary. Assuming the boundary as the energy surface $\Sigma_H = \{H \equiv 1\}$ of a Hamiltonian H, we define H as $H(x) := \frac{1}{\mu^2}$, where $\mu\, x \in \Sigma_H$, $H(0) := 0$. Such an H is strictly convex and positive homogeneous of degree two and we can apply the proposed numerical algorithm. The algorithm yields a periodic solution of the Hamiltonian system (1.2) on $\{H \equiv 1\}$. We know, see Theorem 8, that the period of such a solution equals its action. For each example we give the numerically calculated action of the solution and a figure of the numerical solution. Moreover, we discuss to what extent the numerical solution depends on the chosen starting point and we investigate the dependence on the number of intervals.

Example 1 (continued) We know that the minimal action on ∂C_1 equals $\frac{\pi}{4} \approx 0.785398$. Choosing the number of subintervals as $m = 40$ and the stopping error as 1e−5 (i.e., the iteration stops if the Euclidean norm of the projected gradient is smaller than 1e−5), the program yields after 38 iteration steps as an approximation of the minimal action

$$2\lambda = 0.787018.$$

A decrease of the stopping error only influences the following decimal places. The periodic orbit with minimal action on ∂C_1 is a circle with $r = \frac{1}{2}$ in the (x_2, x_4)-plane. The numerically determined orbit, with $m = 100$, is shown in Figure 3.1.

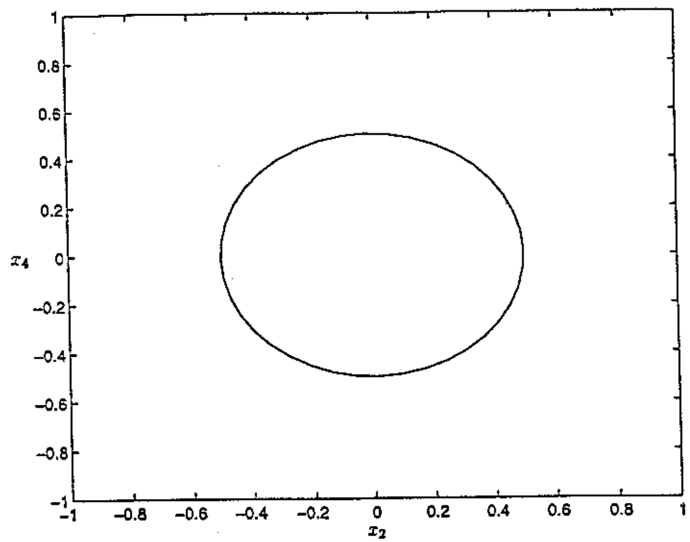

Figure 3.1: *Numerical solution of Example 1*

Example 2 (continued) Recall that the minimal action on ∂C_2 equals $\frac{\pi}{2} \approx 1.570796$. With the same choices as in Example 1 regarding number of subintervals and stopping error, the numerical algorithm yields in 20 iteration steps as an approximation of the minimal action

$$2\lambda = 1.605924.$$

The periodic orbit with minimal action on ∂C_2 is a circle with $r = \frac{1}{\sqrt{2}}$ in the (x_2, x_4)-plane. In Figure 3.2 the orbit obtained by the algorithm (with 100 subintervals) is shown.

Example 3 (continued) We found the lower bound 2.697 and the upper bound 3.586 for the minimal action on ∂C_3. Choosing the same number of subintervals and the same stopping error as in the examples above, we obtain via the numerical program within 29 iteration steps

$$2\lambda = 2.981227$$

as an approximation of the minimal action on ∂C_3. The part of the obtained periodic orbit in the (x_1, x_3)-plane is plotted in Figure 3.3 and the part in the (x_2, x_4)-plane in Figure 3.4.

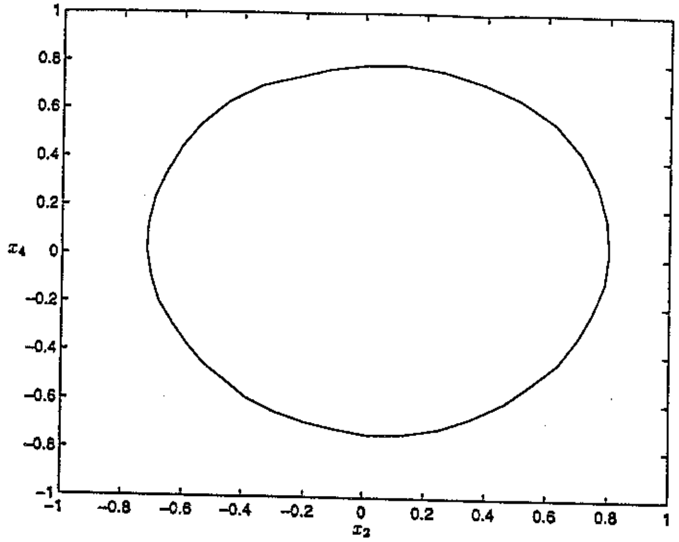

Figure 3.2: *Numerical solution of Example 2*

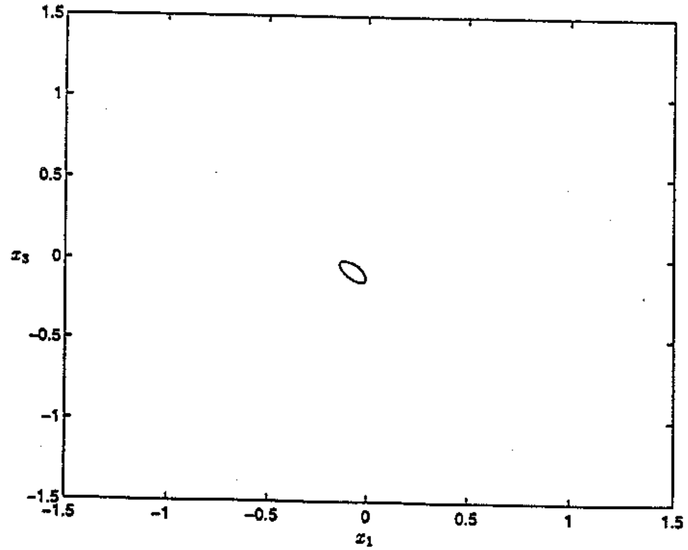

Figure 3.3: *Numerical solution of Example 3 in* (x_1, x_3)*-plane*

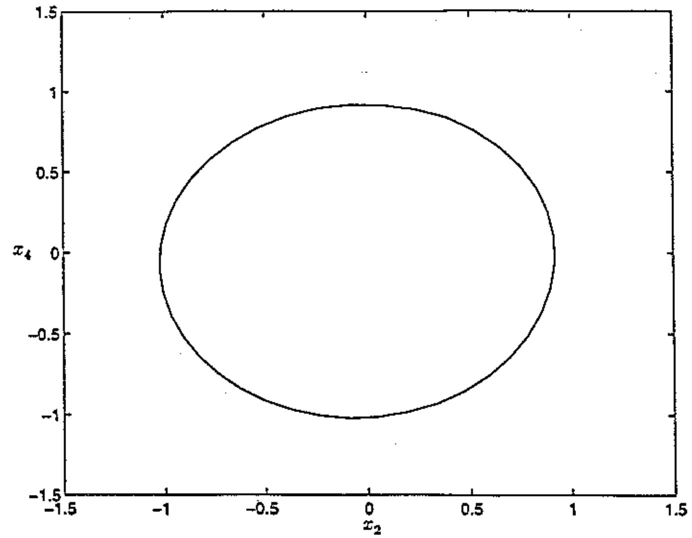

Figure 3.4: *Numerical solution of Example 3 in* (x_2, x_4)*-plane*

Example 4 (continued) On ∂C_4 we know the minimal action is equal to π. With the same choices of subintervals and stopping error as above in 21 iteration steps the algorithm leads to

$$2\lambda = 3.150302$$

as an approximation of the minimal action. This example is different from the others in the sense that on ∂C_4 there are two periodic orbits of the Hamiltonian system with minimal action: a circle with $r = 1$ in the (x_1, x_3)-plane and a circle with $r = 1$ in the (x_2, x_4)-plane. In Figure 3.5 we see a numerical solution obtained by the algorithm, with 100 subintervals. Note that the numerical solution depends on the starting point of the algorithm, see Subsection 3.4.1.

3.4.1 Dependence on the Starting Point

We investigate the dependence of the algorithm on starting points with Example 2 and Example 4. As pointed out, in contrast to Example 2 in Example 4, there are two different periodic orbits of minimal action of

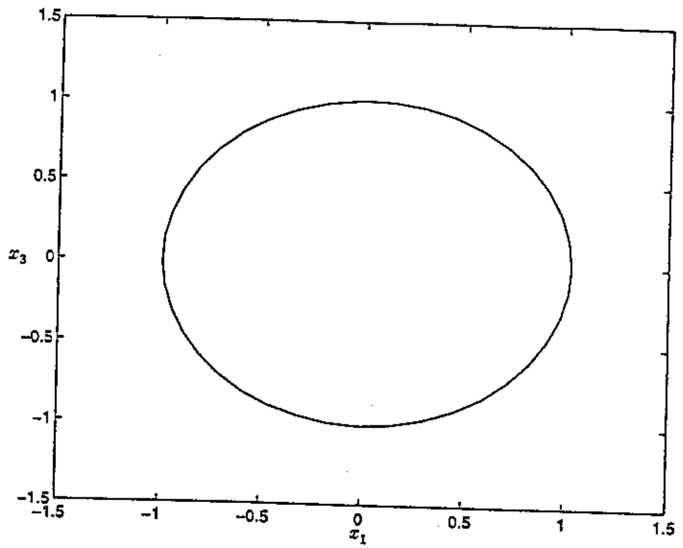

Figure 3.5: *Numerical solution of Example 4*

the Hamiltonian system (1.2) on the energy surface $\{H \equiv 1\}$. Consider Example 2. If we start the algorithm in an arbitrary point $x \in (\mathbb{R}^4)^m$ we obtain the solution of minimal action in the (x_2, x_4)-plane. Whereas, when we start in a point $y = (y_0^{(1)}, \dots, y_0^{(4)}, \dots, y_{m-1}^{(1)}, \dots, y_{m-1}^{(4)}) \in (\mathbb{R}^4)^m$ with $y_i^{(2)} = y_i^{(4)} = 0$ for all $0 \le i \le m-1$, then during all iteration steps of the algorithm the iteration points stay in the (x_1, x_3)-plane. Hence, the periodic orbit obtained lies in the (x_1, x_3)-plane and is a circle with $r = 1$. We remark that as soon as for one i, $0 \le i \le m-1$, the coordinate $x_i^{(2)}$ or $x_i^{(4)}$ is different from 0, the algorithm leads to the periodic orbit with minimal action.

Now consider Example 4. Which periodic orbit is determined by the numerical algorithm depends on the starting point. If the algorithm is started in a point $y = (y_0^{(1)}, \dots, y_0^{(4)}, \dots, y_{m-1}^{(1)}, \dots, y_{m-1}^{(4)}) \in (\mathbb{R}^4)^m$ with $\|(y_0^{(2)}, y_0^{(4)}, y_1^{(2)}, y_1^{(4)}, \dots, y_{m-1}^{(2)}, y_{m-1}^{(4)})\|$ "small", then the algorithm yields the periodic orbit with minimal action in the (x_1, x_3)-plane. Analogously, the periodic orbit with minimal action in the (x_2, x_4)-plane is obtained. As a special case we consider a starting point in the plane with $(x_1 = x_2, x_3 = x_4)$, the "diagonal". If the stopping error is chosen

m	Approx.
5	0.9081781
10	0.8122993
20	0.7919579
40	0.7870181
80	0.7859872
	0.7853981 ($\frac{\pi}{4}$)

Table 3.1: *Example 1: Approximation of the minimal action depending on the number m of subintervals. True value: $\frac{\pi}{4}$.*

not too small, 1e−3 say, the algorithm finds a periodic solution of the Hamiltonian system (1.2), not having minimal action. That is, the algorithm finds a solution of the minimization problem which is a local and not a global minimum. Looking at this solution in the (x_1, x_3)-plane as well as in the (x_2, x_4)-plane, in each case it is a circle with $r = (\frac{1}{2})^{\frac{1}{4}}$. Whereas, if the stopping error is chosen very small, i.e. the number of iteration steps increases, the iteration glides either in the direction of the (x_1, x_3)-plane or the (x_2, x_4)-plane and then one of the two periodic orbits with minimal action is obtained.

3.4.2 Dependence on the Number of Subintervals

Considering Example 1 and Example 4 we investigate how the algorithm depends on the number m of subintervals. For each chosen m the results are shown in Table 3.1 and Table 3.2.

Denote the approximation of the minimal action with m chosen by $2\,\lambda_m$ and the exact minimal action by $2\lambda_{exact}$, then we derive from Tables 3.1 and 3.2 the relationship

$$\lambda_m - \lambda_{exact} \approx \frac{c}{m^2}$$

with a constant c. Hence we deduce that the error is of order 2

$$\lambda_m = \lambda_{exact} + O(m^{-2}),$$

m	Approx.
5	3.6150880
10	3.2547078
20	3.1736357
40	3.1502321
80	3.1440204
	3.1415927 (π)

Table 3.2: *Example 4: Approximation of the minimal action depending on the number m of subintervals. True value: π.*

and

$$\frac{\lambda_{\frac{m}{2}} - \lambda_{exact}}{\lambda_m - \lambda_{exact}} \approx 4,$$

i.e., doubling the number m of subintervals we reduce four times the amount of the difference between the approximation and the exact minimal action.

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