Numerical Continuation of Hamiltonian Relative Periodic Orbits

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Abstract

The bifurcation theory and numerics of periodic orbits of general dynamical systems is well developed, and in recent years there has been rapid progress in the development of a bifurcation theory for dynamical systems with structure, such as symmetry or symplecticity. But as yet there are few results on the numerical computation of those bifurcations. The methods we present in this paper are a first step towards a systematic numerical analysis of generic bifurcations of Hamiltonian symmetric periodic orbits and relative periodic orbits (RPOs). First we show how to numerically exploit spatio-temporal symmetries of Hamiltonian periodic orbits. Then we describe a general method for the numerical computation of RPOs persisting from periodic orbits in a symmetry breaking bifurcation. Finally we present an algorithm for the numerical continuation of non-degenerate Hamiltonian relative periodic orbits with regular drift-momentum pair. Our pathfollowing algorithm is based on a multiple shooting algorithm for the numerical computation of periodic orbits via an adaptive Poincaré section and a tangential continuation method with implicit reparametrization. We apply our methods to continue the famous Figure Eight choreography of the three-body system. We find a relative period doubling bifurcation of the planar rotating Eight family and compute the rotating choreographies bifurcating from it.

AMS subject classification. 37G15, 37J20, 37M20, 70H33
Keywords. Numerical continuation, symmetric Hamiltonian systems, relative periodic orbits.

Short title: Numerics of Hamiltonian relative periodic orbits

Contents

1 Introduction

The numerical bifurcation analysis of periodic orbits of general systems is well-developed, see e.g. [21] and references therein. Today's challenges include the computation of periodic orbits of partial differential equations, the computation of homoclinic orbits and nearby periodic orbits, and the computation of degenerate periodic orbits of high codimension. One example where highly degenerate periodic orbits show up generically are symmetric Hamiltonian systems. This is due to the existence of various conservation laws enforced by symmetry which change the generic behaviour of periodic orbits dramatically. The development of a theory which classifies all generic local bifurcations of periodic and relative periodic orbits in symmetric Hamiltonian

systems and the parallel development of numerical methods for the computation of those bifurcations are open problems, and the current paper is a contribution towards their solution.

Relative periodic orbits are ubiquitous in symmetric Hamiltonian systems. For example generalizations of the Moser-Weinstein theorem show that they occur near any stable relative equilibrium [31]. Specific examples where relative periodic orbits have been discussed or could be found near relative equilibria include gravitational N-body problems, molecules, underwater vehicles, vortices in ideal fluids and continuum mechanics, see e.g. [4, 25, 26, 28, 34, 37] and the references therein. A relative equilibrium is an equilibrium after symmetry reduction, and a relative periodic orbit (RPO) is a trajectory which is periodic after symmetry reduction. Hence RPOs are a natural generalization of periodic orbits in non-symmetric systems. In the case of rotational symmetry an RPO becomes periodic in an appropriate corotating frame and is in general a quasiperiodic solution in the original coordinates. If the symmetry group is discrete then an RPO is a periodic orbit, but its relative period (the period of the corresponding periodic orbit in the space of group orbits) is a fraction of the period of the orbit. In other words, the periodic orbit has in general some spatio-temporal symmetry, for more details see Section 2.

A general theory of generic local bifurcations of symmetric periodic orbits and RPOs for dissipative systems can be found in [22, 23, 36]. For symmetric Hamiltonian systems such a theory has yet to be developed. Recent progress in the theory of persistence of Hamiltonian RPOs to nearby energy-momentum level sets can be found e.g. in [27, 34]. As a consequence of the lack of a general bifurcation theory of Hamiltonian RPOs the numerical bifurcation analysis of these solutions is also still in its infancy.

It is well known that periodic orbits of Hamiltonian systems can be computed numerically by adding an unfolding parameter to overcome the degeneracy caused by energy conservation, see e.g. [15, 29]. In this paper we are concerned with the numerical continuation of symmetric Hamiltonian periodic orbits and RPOs. We show how to numerically exploit spatio-temporal symmetries in the computation of Hamiltonian periodic orbits by extending corresponding methods for dissipative systems [38] to Hamiltonian systems. Moreover, in the case of continuous symmetries, we compute symmetry breaking bifurcations of relative periodic orbits from periodic orbits and show how to continue non-degenerate RPOs of compact group actions in the conserved quantities momentum and energy, building on the persistence results from [34]. We use the methods of unfolding parameters of Muñoz-Almaraz et al [15, 29], but whereas Muñoz-Almaraz et al [15, 29] continue Hamiltonian periodic orbits in external parameters we focus on continuation in internal parameters, namely the conserved quantities of the Hamiltonian system. The main issue here is to specify how unfolding parameters have to be added in order to compute the whole manifold of nearby RPOs without computing symmetry-conjugate solutions. In this approach the exploitation of discrete spatio-temporal symmetries of the periodic orbits and RPOs is essential.

In this paper we do not consider reversing symmetries, but instead develop methods which are applicable to general, not necessarily reversible Hamiltonian systems and can be used to continue non-reversible periodic orbits of reversible systems. We note that, if the periodic orbits to be continued are required to be reversible, then other methods are available which exploit the reversing symmetry and do not require the introduction of unfolding parameters, cf [4, 30].

We apply our results to the three-body problem in celestial mechanics. There is a vast literature on this topic. Periodic orbits of the restricted three-body problem were numerically computed by the Copenhagen team in the early 20th century, see e.g. [3]. Since then periodic orbits of the restricted and full three-body problem have been the subject of various numerical investigations, see e.g. [7, 8, 9, 18, 19, 25] and references therein. Chenciner and Montgomery [6] proved the existence of a new type of periodic orbit of the three-body problem, namely the Figure Eight choreography. Choreographies are special periodic orbits of the N-body system for which all bodies travel along the same curve in configuration space. Many other choreographies have

been found numerically by Simó et al [5, 33]. The Figure Eight choreography has been continued, with respect to the mass of the bodies, by Galán et al [15]. We numerically compute three families of relative periodic orbits which bifurcate from the famous Figure Eight choreography to non-zero angular momentum. These families have been found numerically by Marchal [25], Chenciner et al and Hénon respectively, see [4]. The existence of these rotating choreographies has been proved by Chenciner et al [4]. They continue the rotating Figure Eight solutions numerically by exploiting their reversibility. As mentioned above, we do not consider reversing symmetries, but we reprove the result in [4] on the existence of rotating Eights using reduced Poincaré maps rather than Lyapunov-Schmidt reduction on loop spaces as in [4]. We generalize it to N bodies and characterize it as special case of a persistence result for RPOs from [34]. Moreover, our existence proof directly implies convergence of the corresponding numerical method. Applying our numerical methods to the Figure Eight we find a relative period doubling bifurcation along the branch of planar rotating Eights and compute the bifurcating branch.

The paper is organized as follows: In Section 2 we extend the numerical continuation techniques for symmetric periodic orbits of general systems which we developed in [38] to Hamiltonian systems. Then, in Section 3, we consider systems with continuous symmetry groups and continuation of relative periodic orbits. In particular, we review our persistence results for non-degenerate relative periodic orbits with regular drift-momentum pair [34] and present an algorithm for the continuation of such relative periodic orbits. In Section 4 we apply our numerical methods to rotating choreographies in the three-body problem.

Acknowledgements

CW was partially supported by the Nuffield Foundation, by a European Union Marie Curie fellowship under contract number HPMF-CT-2000-00542 and by an EPSRC First Grant. We thank Mark Roberts for stimulating discussions and for suggesting to apply our numerical continuation methods to the Figure Eight solution of the three-body problem. CW thanks the Freie Universität Berlin, and in particular the research group of Bernold Fiedler, for their hospitality during visits when parts of this paper were written. Finally we thank Frank Schilder for his useful comments on the paper.

2 Numerical continuation of symmetric Hamiltonian periodic orbits

In this section we show how symmetric periodic orbits of Hamiltonian systems can be continued numerically with respect to energy and how spatio-temporal symmetries can be exploited. We extend the numerical methods presented in [38] for dissipative systems to Hamiltonian systems.

2.1 Periodic orbits of Hamiltonian systems

Mechanical systems arising for example in celestial mechanics or molecular dynamics are examples of Hamiltonian systems [1, 26]. A Hamiltonian system is given by

$$\dot{x} = f_H(x) = \mathbb{J}\nabla H(x), \quad x \in X \tag{2.1}$$

where X is an open subset of $\mathbb{R}^n$. Here $n = 2d$ is even, $H : X \to \mathbb{R}$ is called the *Hamiltonian* or *energy* of the system, $\mathbb{J} \in \mathrm{Mat}(n)$ is a skew-symmetric, invertible matrix and $\nabla H = (\mathrm{D}H)^T$ is the column vector containing the gradient of H. The inverse $\mathbb{J}^{-1}$ of $\mathbb{J}$ is called the *symplectic structure matrix* and defines the *symplectic form*

$$\omega(v, w) = \langle v, \mathbb{J}^{-1} w \rangle. \tag{2.2}$$

The Hamiltonian vectorfield f_H from (2.1) is then defined by

$$\omega(f_H(x), w) = \mathrm{D}H(x)w, \quad x \in X, w \in \mathbb{R}^n.$$

In many applications $\mathbb{J}$ is given by

$$\mathbb{J} = \begin{pmatrix} 0 & \mathrm{id}_d \\ -\mathrm{id}_d & 0 \end{pmatrix}, \tag{2.3}$$

and x takes the form $x = (q, p)$ with $q \in \mathbb{R}^d$ and $p \in \mathbb{R}^d$. Then q is called the position and p the momentum variable. We can then rewrite (2.1) in the equivalent form

$$\dot{q} = \nabla_p H(p, q), \quad \dot{p} = -\nabla_q H(p, q).$$

One can easily check that solutions $x(t)$ of a Hamiltonian system (2.1) conserve the energy:

$$\frac{\mathrm{d}}{\mathrm{d}t} H(x(t)) = \mathrm{D}H(x(t))\dot{x}(t) = \mathrm{D}H(x(t))\mathbb{J}\nabla H(x(t)) = 0.$$

Let $\bar{x} = x(0)$ lie on a $\bar{T}$-periodic orbit $\bar{\mathcal{P}} = \{x(t), t \in \mathbb{R}\}$, i.e., $x(\bar{T}) = x(0)$ or equivalently $\Phi_{\bar{T}}(\bar{x}) = \bar{x}$ where Φ_t is the flow of (2.1). With $x(t)$ also $x(t+t_0)$, $t_0 \in \mathbb{R}$, is a periodic solution of (2.1). To eliminate this non-uniqueness caused by time shift symmetry we fix a section $S = S_{\bar{x}}$ transverse to the periodic orbit at $\bar{x}$ (a Poincaré section), e.g.

$$S = \bar{x} + \mathrm{span}(f_H(\bar{x}))^{\perp}, \tag{2.4}$$

and consider the first return map $\Pi : S \to S$ from S to S. Then Π is called Poincaré map, see e.g. [1]. As a consequence of energy conservation, in the case of Hamiltonian systems the derivative $\mathrm{D}_x\Pi(\bar{x})$ of the Poincaré map $\Pi : S \to S$ at $\bar{x} = x(0)$ always has an eigenvalue 1: Since $H(x) = H(\Phi_t(x))$ for all $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, we have

$$\mathrm{D}H(x) = \mathrm{D}H(\Phi_t(x))\mathrm{D}_x\Phi_t(x). \tag{2.5}$$

Thus, in the periodic orbit we get

$$\mathrm{D}H(\bar{x})(\mathrm{D}_x\Phi_{\bar{T}}(\bar{x}) - \mathrm{id}) = 0. \tag{2.6}$$

Furthermore

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\Phi_t(\bar{x})) = 0 \implies \mathrm{D}H(\bar{x})f(\bar{x}) = 0, \tag{2.7}$$

so that $\mathrm{D}H(\bar{x})$ lies in the dual of the tangent space of the Poincaré section S and so is a left eigenvector of $\mathrm{D}_x\Pi(\bar{x})$ to the eigenvalue 1. We therefore restrict the Poincaré section to

$$S^{\bar{E}} := S \cap X^{\bar{E}},$$

where

$$X^{\bar{E}} = \{x,\ H(x) = \bar{E}\}$$

is the energy level set of the periodic orbit ($\bar{E} = H(\bar{x})$) and consider the Poincaré map $\Pi^{\bar{E}} : S^{\bar{E}} \to S^{\bar{E}}$ inside this energy-level set. We can, without loss of generality, assume that $\bar{E} = 0$.

Definition 2.1 *We call a periodic solution $x(t)$ of a Hamiltonian system (2.1) through $\bar{x} = x(0)$* non-degenerate *if it is a non-degenerate periodic solution inside its energy level $X^{\bar{E}}$, i.e., if it is a proper periodic solution (not an equilibrium) and if*

$$\mathrm{D}\Pi^{\bar{E}}(\bar{x}) - \mathrm{id}$$

is invertible.

If $\bar{\mathcal{P}}$ is a non-degenerate periodic orbit then 1 is a single eigenvalue of the derivative of the Poincaré map $\mathrm{D}_x\Pi(\bar{x})$ at $\bar{x} \in \bar{\mathcal{P}}$. In this case there is a two-dimensional manifold $\mathcal{P}(E)$ of periodic orbits parametrized by energy such that $\mathcal{P}(\bar{E}) = \bar{\mathcal{P}}$, see [1]. The non-degeneracy condition is generically satisfied.

2.2 Hamiltonian systems with discrete symmetries

We now assume that the Hamiltonian H of the Hamiltonian system (2.1) is invariant under a finite group $\Gamma \subseteq \mathrm{GL}(n)$:

$$H(x) = H(\gamma x) \quad \text{for all} \quad \gamma \in \Gamma \tag{2.8}$$

and that Γ acts symplectically, i.e.,

$$\Gamma \subseteq \mathrm{SP}(n)$$

where $\mathrm{SP}(n)$ is the *symplectic group*

$$\mathrm{SP}(n) = \{\gamma \in \mathrm{GL}(n), \quad \gamma^T \mathbb{J}^{-1} \gamma = \mathbb{J}^{-1}\}.$$

We also assume that the action of Γ on $\mathbb{R}^n$ is faithful. Under these assumptions the Hamiltonian vectorfield f_H from (2.1) is Γ-equivariant, i.e., it commutes with Γ:

$$f_H(\gamma x) = \gamma f_H(x) \quad \forall \gamma \in \Gamma, x \in X.$$

This condition on the vectorfield (2.1) implies that if $x(t)$ is a solution of the dynamical system (2.1) then also $\gamma\, x(t)$ is a solution. Hence the flow $\Phi_t(\cdot)$ of (2.1) is Γ-equivariant as well: $\Phi_t(\gamma x) = \gamma \Phi_t(x)$ for all γ, x, t.

An element $\gamma \in \Gamma$ is called a *symmetry* of $\bar{x} \in \mathbb{R}^n$ if $\gamma \bar{x} = \bar{x}$; the set of all symmetries of $\bar{x}$ (*isotropy subgroup* of $\bar{x}$) is given by $K = \Gamma_{\bar{x}} = \{\gamma \in \Gamma \mid \gamma \bar{x} = \bar{x}\}$. The *spatial symmetries* K of periodic solutions $x(t)$ are those group elements $\gamma \in \Gamma$ which leave each point on the periodic orbit invariant:

$$K := \Gamma_{x(t)} = \{\gamma \in \Gamma \mid \gamma x(t) = x(t) \quad \text{for all} \quad t \in \mathbb{R}\}.$$

Since the flow Φ_t is Γ-equivariant the set of spatial symmetries K of a periodic solution $x(t)$ does not depend on the time t. In addition to spatial symmetries there are also *spatio-temporal symmetries* which leave the periodic orbit $\bar{\mathcal{P}} := \{x(t), t \in \mathbb{R}\}$ invariant as a whole but not pointwise: The spatio-temporal symmetries of a periodic orbit $\bar{\mathcal{P}}$ are given by

$$L := \{\gamma \in \Gamma \mid \gamma \bar{\mathcal{P}} = \bar{\mathcal{P}}\}.$$

Each $\gamma \in L$ corresponds to a phase shift $\Theta(\gamma)\, \bar{T}$ of the $\bar{T}$-periodic solution $x(t)$:

$$\gamma \in L \Rightarrow x(t) = \gamma x(t + \Theta(\gamma)\, \bar{T}), \text{ where } \Theta(\gamma) \in S^1 \simeq \mathbb{R}/\mathbb{Z}. \tag{2.9}$$

So spatio-temporal symmetries come in pairs $(\gamma, \Theta(\gamma)) \in \Gamma \times S^1$. We define an action of the spatio-temporal symmetry group $\Gamma \times S^1$ on $\bar{T}$-periodic solutions $x(t)$ of (2.1) as follows:

$$((\gamma, \theta)x)(t) := \gamma x(t + \theta \bar{T}), \quad (\gamma, \theta) \in \Gamma \times S^1. \tag{2.10}$$

Note that $\Theta : L \to S^1$ is a group homomorphism with the spatial symmetries K as kernel and that K is normal in L such that

$$L/K \equiv \mathbb{Z}_\ell \quad \text{for some} \quad \ell \in \mathbb{N}, \tag{2.11}$$

see [17].

Remark 2.2 It can be seen easily that the vectorfield f_H of (2.1) maps the fixed point space of K in X

$$X_{\mathrm{red}} := \mathrm{Fix}_X(K) = \{x \in X \mid \gamma x = x \, \forall \gamma \in K\}$$

into itself. Thus we can restrict the differential equation (2.1) to the fixed point space X_{red} which has a lower dimension $n_{\mathrm{red}} \leq n$. This way we obtain a symmetry reduced system f_{red} :

$X_{\rm red} \to \mathbb{R}^{n_{\rm red}}$ which can be computed symbolically (see Gatermann and Hohmann [16]). By restriction onto the fixed point space $\mathrm{Fix}_X(K)$ the spatial symmetries of periodic solutions can be exploited. The symmetry reduced system $f_{\rm red} : X_{\rm red} \to \mathbb{R}^{n_{\rm red}}$ has symmetry group $N(K)/K$ where $N(K)$ is the normalizer of K.

From now on we assume, unless stated otherwise, that the spatial symmetry K of the periodic orbit is trivial by replacing the phase space by $\mathrm{Fix}_X(K)$ and the symmetry group Γ of the Hamiltonian system (2.1) by $N(K)/K$. The spatio-temporal symmetries of the periodic orbit then form a finite cyclic group $L = \mathbb{Z}_\ell$.

In bifurcation theory the spatio-temporal symmetry of periodic orbits is taken into account by studying the *reduced Poincaré map*. It was first introduced by Fiedler [14]. Despite being easy, this concept is essential for the classification of generic symmetry breaking bifurcations of periodic orbits of general systems, see [22, 23], and for the design of numerical methods for the computation of these bifurcations. Let $\alpha \in L = \mathbb{Z}_\ell$ be that element in L that corresponds to the smallest possible non-zero phase shift $\bar{T}/\ell$:

$$\alpha\, x\left(t + \frac{\bar{T}}{\ell}\right) = x(t) \quad \forall\, t. \tag{2.12}$$

We call this spatio-temporal symmmetry the *drift symmetry* of the periodic orbit $\bar{\mathcal{P}}$, c.f. [34]. For $\bar{x} \in \bar{\mathcal{P}}$ define the Poincaré section as before by $S = \bar{x} + \mathrm{span}(f(\bar{x}))^\perp$. Then the *reduced Poincaré map* $\Pi_{\rm red} : S \to S$ is defined as

$$\Pi_{\rm red} = \alpha\hat{\Pi}, \quad \hat{\Pi} : S \to \alpha^{-1}\, S. \tag{2.13}$$

Here α is the drift symmetry of the periodic orbit and $\hat{\Pi}$ maps $x \in S$ into the point where the positive semi-flow through x first hits $\alpha^{-1}\, S$, see [14]. From (2.8) we get

$$\mathrm{D}H(\gamma x)\gamma = \mathrm{D}H(x) \quad \text{for all } \gamma \in \Gamma, \tag{2.14}$$

and this, together with (2.5), implies that

$$\mathrm{D}H(\bar{x})(\alpha \mathrm{D}_x \Phi_{\frac{\bar{T}}{\ell}}(\bar{x}) - \mathrm{id}) = \mathrm{D}H(\alpha\Phi_{\bar{T}/\ell}(\bar{x}))\alpha \mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{D}H(\bar{x}) = 0. \tag{2.15}$$

Hence, because of (2.7), $\nabla H(\bar{x})$ is a left eigenvector of the reduced Poincaré map $\Pi_{\rm red}$, as in the case of non-symmetric Hamiltonian systems, cf. (2.6). As before, let $\Pi_{\rm red}^{\bar{E}} : S^{\bar{E}} \to S^{\bar{E}}$ be the Poincaré map inside the energy level set $X^{\bar{E}}$ of the periodic orbit ($\bar{E} = H(\bar{x})$).

Definition 2.3 *Analogously to Definition 2.1 we call a symmetric periodic orbit of a Hamiltonian system through $\bar{x}$ non-degenerate if it is not an equilibrium and if*

$$\mathrm{D}\Pi_{\rm red}^{\bar{E}}(\bar{x}) - \mathrm{id}$$

is invertible.

If $\bar{x}$ lies on a non-degenerate symmetric periodic orbit $\bar{\mathcal{P}}$, then there is a one-parameter family $\mathcal{P}(E)$, $E \approx \bar{E}$, of periodic orbits parametrized by energy E closeby which have the same spatio-temporal symmetry as the original periodic orbit $\bar{\mathcal{P}} = \mathcal{P}(\bar{E})$.

2.3 Numerical continuation of symmetric Hamiltonian periodic orbits

In this section we show how symmetric periodic orbits of Hamiltonian systems can be computed numerically.

2.3.1 Single shooting approach

A symmetric periodic orbit of a Γ-equivariant dissipative system $\dot{x} = f(x)$ with drift symmetry $\alpha \in \Gamma$ of order ℓ can be computed as solution of the following underdetermined system (see [10, 38])

$$F(x,T) = \alpha\Phi_{T/\ell}(x) - x = 0. \tag{2.16}$$

Here $\Phi_t(x)$ is the flow of (2.1). If $\mathrm{D}F(\bar{x},\bar{T})$ has full rank in the solution $(\bar{x},\bar{T})$ then the equation $F(y) = 0$ where $y = (x,T)$ can be solved by a Gauss-Newton method [10, 38]:

$$\begin{aligned} \Delta y^k &= -\mathrm{D}F(y^k)^+ F(y^k), \\ y^{k+1} &= y^k + \Delta y^k. \end{aligned} \tag{2.17}$$

Here $\mathrm{D}F(y^k)^+$ denotes the Moore-Penrose pseudo-inverse of $\mathrm{D}F(y^k)$. Remember that for $A \in \mathrm{Mat}(m,n)$, $m \le n$, $\mathrm{rank}\ A = m$, $x \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, $x = A^+ b$ is defined by

$$Ax = b, \quad x \perp \ker(A).$$

Here $\ker(A)$ denotes the kernel of A. The Jacobian $\mathrm{D}F(x,T)$ of (2.16) in the solution $(\bar{x},\bar{T})$ is given by

$$\mathrm{D}F(\bar{x},\bar{T}) = [\alpha \mathrm{D}_x\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}, \frac{1}{\ell}\alpha f(\Phi_{\bar{T}/\ell}(\bar{x}))] = [\alpha \mathrm{D}_x\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}, \frac{1}{\ell} f(\bar{x})]. \tag{2.18}$$

Equation (2.12) implies that

$$(\alpha \mathrm{D}_x\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}) f_H(\bar{x}) = 0. \tag{2.19}$$

Therefore a kernel vector t^f of $\mathrm{D}F(\bar{y})$ at the solution point $\bar{y} = (\bar{x},\bar{T})$ is the tangent $t^f = (f(\bar{x}),0)$ to the trajectory.

Remark 2.4 This approach can be interpreted as computing periodic orbits in an *adaptive Poincaré section*, which is *approximately orthogonal* to the periodic orbit: Since for the kernel vectors $t^k = (t_x^k, t_T^k)$ of $\mathrm{D}F(y^k)$ we have $t^k \to t^f$ as $k \to \infty$, the Gauss-Newton iterate $x^{k+1} = x^k + \Delta x^k$ lies in the adaptive Poincaré section $S_{x^k} = x^k + \mathrm{span}(t_x^k)^\perp \approx \bar{x} + \mathrm{span}(f(\bar{x}))^\perp$.

Periodic orbits of Hamiltonian systems can not be computed numerically by solving (2.16) because, due to conservation of energy, the Jacobian $\mathrm{D}F$ is singular in every solution of (2.16) with rank defect (at least) one. This follows from the fact that in a solution point $(\bar{x},\bar{T})$ of (2.16) we have, by (2.18), (2.7) and (2.15), that

$$\begin{aligned} \mathrm{D}H(\bar{x})\mathrm{D}F(\bar{x},\bar{T}) &= \mathrm{D}H(\bar{x})[\alpha \mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}, \ \frac{1}{\ell} f_H(\bar{x})] \\ &= [\mathrm{D}H(\bar{x})(\alpha \mathrm{D}_x\Phi_{\frac{\bar{T}}{\ell}}(\bar{x}) - \mathrm{id}), \frac{1}{\ell}\mathrm{D}H(\bar{x}) f_H(\bar{x})] \\ &= 0. \end{aligned}$$

Periodic orbits of Hamiltonian systems are usually computed by adding an unfolding term so that (2.1) becomes a one-parameter family of vectorfields, see e.g. [15, 29, 35]: we consider the ordinary differential equation

$$\dot{x} = f(x,\lambda) = f_H(x) + \lambda \nabla H(x). \tag{2.20}$$

For any solution $x(t)$ of (2.20) we have

$$\frac{\mathrm{d}}{\mathrm{d}t} H(x(t)) = \mathrm{D}H(x(t))(f_H(x(t)) + \lambda \nabla H(x(t)) = \lambda \|\nabla H(x(t))\|^2. \tag{2.21}$$

So if $x(t)$ is non-stationary then $H(x(t))$ is strictly monotone in t if $\lambda \neq 0$. Since for a T-periodic solution $x(t)$ of (2.20) we have $H(x(0)) = H(x(T))$ it follows that $\lambda = 0$. We can therefore compute symmetric periodic orbits by solving

$$0 = F(y) = F(x, T, \lambda) = \alpha\Phi_{T/\ell}(x; \lambda) - x \tag{2.22}$$

where $\Phi_t(\cdot; \lambda)$ is the flow of (2.20). Moreover we have the following convergence theorem which generalizes corresponding results in [15, 29, 35] to periodic orbits with spatio-temporal symmetry:

Theorem 2.5 *The Jacobian*

$$\mathrm{D}F(\bar{x}, \bar{T}, \lambda)|_{\lambda=0} = [\alpha \mathrm{D}_x \Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}, \quad \frac{1}{\ell} f_H(\bar{x}), \quad \alpha \mathrm{D}_\lambda \Phi_{\bar{T}/\ell}(\bar{x})] \tag{2.23}$$

of (2.22) is regular in the solution point $(\bar{x}, \bar{T}, 0)$ if the $\bar{T}$-periodic orbit $\bar{\mathcal{P}}$ through $\bar{x}$ is non-degenerate in the sense of Definition 2.3. In this case the Gauss-Newton method (2.17) applied to (2.22) with $y = (x, T, \lambda)$ converges to a periodic orbit on the path of periodic orbits $\mathcal{P}(E)$ near $\bar{\mathcal{P}} = \mathcal{P}(\bar{E})$ for sufficiently close initial data $\hat{y} \approx (\bar{\mathcal{P}}, \bar{T}, 0)$.

Proof. We check that the Jacobian $\mathrm{D}F(x, T, \lambda)|_{\lambda=0}$ has full rank in every solution point $(\bar{x}, \bar{T}, 0)$, $\bar{x} \in \bar{\mathcal{P}}$. We have

$$\begin{aligned}
\mathrm{D}H(\bar{x})\mathrm{D}_\lambda F(\bar{x}, \bar{T}, \bar{\lambda})|_{\bar{\lambda}=0} &= \mathrm{D}H(\bar{x})\alpha \mathrm{D}_\lambda \Phi_{\bar{T}/\ell}(\bar{x}; \bar{\lambda})|_{\bar{\lambda}=0} \\
&= \mathrm{D}_\lambda H(\alpha\Phi_{\bar{T}/\ell}(\bar{x}; \bar{\lambda}))|_{\bar{\lambda}=0} \\
&= \mathrm{D}_\lambda H(\Phi_{\bar{T}/\ell}(\bar{x}; \bar{\lambda}))|_{\bar{\lambda}=0} \\
&= \mathrm{D}_\lambda \textstyle\int_0^{\bar{T}/\ell} \frac{\mathrm{d}}{\mathrm{d}t} H(\Phi_t(\bar{x}; \bar{\lambda}))\mathrm{d}t|_{\bar{\lambda}=0} \\
&= \mathrm{D}_\lambda \textstyle\int_0^{\bar{T}/\ell} \lambda \|\nabla H(\Phi_t(\bar{x}; \bar{\lambda}))\|^2 \mathrm{d}t|_{\bar{\lambda}=0} \\
&= \textstyle\int_0^{\bar{T}/\ell} \|\nabla H(\Phi_t(\bar{x}))\|^2 \mathrm{d}t \neq 0.
\end{aligned} \tag{2.24}$$

Here we used the Γ-invariance of H (see (2.8)) in the third line, and (2.21) in the fifth line. From (2.23) and (2.24) we conclude that in a non-degenerate periodic orbit $\mathrm{D}F(\bar{x}, \bar{T}, 0)$ has full rank. The solution manifold of $F = 0$ is therefore two-dimensional and locally given by the two-dimensional manifold $\{\mathcal{P}(E),\ E \approx \bar{E}\}$. ∎

Remark 2.6 Note that $\mathrm{D}F(\bar{x}, \bar{T}, 0)$ also has full rank and our numerical method converges if $\bar{x}$ lies on a degenerate periodic orbit which is a turning point with respect to energy continuation.

Remark 2.7 If a simple parametrization of constant energy level sets near the periodic orbit is explicitly available then the number of variables could be reduced by one and the introduction of an unfolding parameter would not be necessary. In general, such parametrizations are not easily available. We therefore prefer the widely used method described above, where additional unfolding parameters are introduced to take into account the energy conservation. Existing powerful continuation methods for periodic orbits, see e.g. [15, 29, 38] and references therein, are readily applicable in our approach.

2.3.2 Continuation with respect to energy

At a non-degenerate symmetric periodic orbit the equation

$$\mathcal{F}(x, E) = 0, \quad \text{where } \mathcal{F}(x, E) : S^E \times \mathbb{R} \to S^E \text{ is given by } \mathcal{F}(x, E) = \Pi^E_{\mathrm{red}}(x) - x, \tag{2.25}$$

depends smoothly on E and can be solved by the implicit function theorem. Its solutions $x(E)$ lie on symmetric periodic orbits $\mathcal{P}(E)$ with energy E. In [13] a tangential continuation method based on implicit reparametrization is presented to solve systems of the form $f(x,\lambda)=0$, where $f: X\times\mathbb{R}\to\mathbb{R}^n$, $X\subset\mathbb{R}^n$ open. The pathfollowing algorithm works as follows: if a solution $\bar{y}=(\bar{x},\bar{\lambda})$ together with its continuaton tangent $t(\bar{y})$, the kernel vector of $\mathrm{D}_y f(\bar{y})$, are given a new guess point $\hat{y}$ is computed by setting $\hat{y}=\bar{y}+\epsilon t(\bar{y})$ where ϵ is a suitably chosen stepsize. Then an underdetermined Gauss-Newton method as in (2.17) is used for the iteration from the guess $\hat{y}$ back to the solution path. The stepsize control is described in [13].

Remark 2.8 The continuation method of [13], called "Moore-Penrose continuation" in [21], and Keller's widely used pseudoarclength method [20] are based on the same idea, namely, an implicit arc-length parametrization of the solution path. Both require the Newton corrections to lie in hyperplanes which are approximately perpendicular to the tangent of the solution path. The only difference between the two methods is that Moore-Penrose continuation adapts this approximation during the Newton iteration back to the solution path, whereas it remains fixed during the iteration in Keller's method; see [21, Section 10.2] for more details. In both methods the stepsize controls the change of the entire solution object and there is no designated continuation parameter so that fold bifurcations cause no problems.

In principle we can apply this continuation method to (2.25). But numerically we rather want to compute symmetric perodic orbits by using adaptive Poincaré sections, i.e., by solving (2.22), cf. Remark 2.4. The kernel $\mathrm{D}F$ of (2.22) is at least two-dimensional and exactly two-dimensional at non-degenerate periodic orbits, see Theorem 2.5. As continuation tangent $t^E=(t_x^E,t_T^E,t_\lambda^E)$ we choose the kernel vector of $\mathrm{D}F$ which corresponds to the kernel vector $t^{\mathcal{F}}$ of $\mathrm{D}\mathcal{F}$, i.e., we have to require $t_x^E\in S$. As before, see (2.4), we choose $S=\bar{x}+\mathrm{span}(f_H(\bar{x}))^\perp$ at the periodic orbit through $\bar{x}$.

The continuation tangent t^E can then be computed as follows: Let t_x^λ be the generalized eigenvector of $\alpha\mathrm{D}\Phi_{\frac{T}{\ell}}(\bar{x})$ to the eigenvalue 1 which corresponds to the left eigenvector $\mathrm{D}H(\bar{x})$ of $\alpha\mathrm{D}\Phi_{\frac{T}{\ell}}(\bar{x})$, see (2.15), i.e. $\mathrm{D}H(\bar{x})t_x^\lambda\neq 0$. Then there is a constant t_T^λ such that the vector $t^\lambda=(t_x^\lambda,t_T^\lambda,0)$ lies in the kernel of $\mathrm{D}F(\bar{y})$ and is linearly independent of the second kernel vector $t^f=(t_x^f,0,0)$ of $\mathrm{D}F(\bar{y})$ where $t_x^f=f_H(\bar{x})$, see (2.19). Since $\mathrm{D}H(\bar{x})t_x^\lambda\neq 0$ the parameter λ corresponds to a parametrization with respect to energy and we will therefore frequently denote it by λ_E rather than λ in the sequel. The continuation tangent t^E corresponding to $t^{\mathcal{F}}$ is then the kernel vector t^E of $\mathrm{D}F(\bar{y})$ which is orthogonal to t^f.

2.3.3 Fixing the energy

If a periodic orbit with given energy E has to be computed, then we solve the system of equations $F^E(x,T,\lambda_E)=0$ where $F^E: X\times\mathbb{R}^2\subseteq\mathbb{R}^{n+2}\to\mathbb{R}^{n+1}$ is given by

$$F^E(x,T,\lambda_E)=\begin{pmatrix}\alpha\Phi_{\frac{T}{\ell}}(x;\lambda_E)-x\\ H(x)-E\end{pmatrix}. \tag{2.26}$$

Proposition 2.9 *The Jacobian $\mathrm{D}F^{\bar{E}}(\bar{y})$ has full rank in the solution $\bar{y}=(\bar{x},\bar{T},\bar{\lambda}=0)$ if the periodic orbit $\bar{\mathcal{P}}$ through $\bar{x}$ with energy $\bar{E}=H(\bar{x})$ is non-degenerate in the sense of Definition 2.3. In this case the Gauss-Newton method (2.17) applied to $F^E=0$ converges for initial data $\hat{y}\approx(\bar{\mathcal{P}},\bar{T},0)$ and $E\approx\bar{E}$.*

Proof. Note that

$$\mathrm{D}F^{\bar{E}}(\bar{y})=\begin{pmatrix}\alpha\mathrm{D}\Phi_{\frac{\bar{T}}{\ell}}(\bar{x})-\mathrm{id} & \frac{1}{\ell}f_H(\bar{x}) & \alpha\mathrm{D}_\lambda\Phi_{\frac{\bar{T}}{\ell}}(\bar{x})\\ \mathrm{D}H(\bar{x}) & 0 & 0\end{pmatrix}.$$

Due to time shift symmetry and energy conservation the kernel of $\mathrm{D}F(\bar{y})$ with F from (2.22) is at least two-dimensional. If the periodic orbit $\bar{\mathcal{P}} = \mathcal{P}(\bar{E})$ is non-degenerate then, by Theorem 2.5, it is exactly two-dimensional, spanned by t^f and a vector t^E with $\mathrm{D}H(\bar{x})t^E_x \neq 0$. Hence t^E is not in the kernel of $\mathrm{D}F^{\bar{E}}(\bar{y})$ and so $\mathrm{D}F^{\bar{E}}(\bar{y})$ has a one-dimensional kernel and has full rank. The one-dimensional solution manifold of $F^E = 0$ is then given by the periodic orbit $\mathcal{P}(E)$ with energy E. ∎

Remarks 2.10

a) If the Hamiltonian vectorfield depends on an external parameter λ_{ext} then (2.26) becomes dependent on λ_{ext} and can be used to continue non-degenerate periodic orbits with fixed energy in an external parameter.

b) Muñoz-Almaraz et al [15] also use introduce unfolding parameters to deal with energy conservation and continue periodic orbits with fixed period and fixed phase in an external parameter, see Remark 3.26 for more details.

c) If the periodic orbits to be continued are required to be reversible - an additional assumption which we do not impose - then other methods are available which exploit the reversing symmetry and do not require the introduction of unfolding parameters, cf [4, 30].

2.3.4 Multiple shooting ansatz

In order to numerically continue symmetric periodic solutions in numerically delicate situations, that is, when the single shooting method is ill-conditioned, we use the just described algorithm in the *multiple* shooting context, cf. [10, 38]: we compute k points on a periodic orbit with spatio-temporal symmetry $L = \mathbb{Z}_\ell$, trivial isotropy and drift symmetry α by solving the underdetermined equation

$$F(x_1, \ldots, x_k, T, \lambda) = 0, \quad F : X^k \times \mathbb{R}^{q+1} \to \mathbb{R}^M, \tag{2.27}$$

where $X^k \times \mathbb{R}^{q+1} \subseteq \mathbb{R}^N$, $x_j \in X \subseteq \mathbb{R}^n$, $j = 1, \ldots, k$, $T \in \mathbb{R}$, $\lambda \in \mathbb{R}^q$ (in this case $q = 1$), and $N = M + q + 1 = kn + q + 1$. Moreover $0 = s_1 < \ldots < s_{k+1} = 1$ is a partition of the unit interval, $\Delta s_i = s_{i+1} - s_i$ for $i = 1, \ldots k$, and

$$F_i(x_1, \ldots, x_k, T, \lambda) = \begin{cases} \Phi_{\frac{\Delta s_i T}{\ell}}(x_i; \lambda) - x_{i+1} & \text{for} \quad i = 1, \ldots, k-1, \\ \alpha\Phi_{\frac{\Delta s_k T}{\ell}}(x_k; \lambda) - x_1 & \text{for} \quad i = k. \end{cases} \tag{2.28}$$

Remark 2.11 Note that the Gauss Newton method (2.17) applied to (2.27) amounts to using *adaptive integral phase conditions*, c.f. also [10, 21, 38].

The linear systems which arise in the Gauss-Newton method (2.17) are of the form $Jy = b$, where $y = (x, T, \lambda) \in \mathbb{R}^{nk+1+q}$, $x = (x_1, \ldots, x_k)$, $b = (b_1, \ldots, b_k)$, and

$$J = \mathrm{D}F(x, T, \lambda) = \begin{pmatrix} G_1 & -\mathrm{id} & & & & g_1 & p_1 \\ & G_2 & -\mathrm{id} & & & g_2 & p_2 \\ & & \ddots & \ddots & & \vdots & \vdots \\ & & & G_{k-1} & -\mathrm{id} & g_{k-1} & p_{k-1} \\ -\mathrm{id} & & & & G_k & g_k & p_k \end{pmatrix} = [G, g, p]. \tag{2.29}$$

Here G is an (nk, nk)-matrix, g an nk-vector, p an (nk, q)-matrix, and

$$
\begin{aligned}
&G_i = \mathrm{D}_x \Phi_{\frac{\Delta s_i T}{\ell}}(x_i;\lambda), \quad i = 1, 2, \ldots, k-1,\\
&G_k = \alpha \mathrm{D}_x \Phi_{\frac{\Delta s_k T}{\ell}}(x_k;\lambda),\\
&g_i = \mathrm{D}_T F_i(x, T, \lambda) = \mathrm{D}_T \Phi_{\frac{\Delta s_i T}{\ell}}(x_i;\lambda) = \tfrac{\Delta s_i}{\ell} f_H(\Phi_{\frac{\Delta s_i T}{\ell}}(x_i;\lambda), \lambda), \quad i = 1, \ldots, k-1,\\
&g_k = \alpha \tfrac{\Delta s_k}{\ell} f_H(\Phi_{\frac{\Delta s_k T}{\ell}}(x_k;\lambda), \lambda)\\
&p_i = \mathrm{D}_\lambda F_i(x, T) = \mathrm{D}_\lambda \Phi_{\frac{\Delta s_i T}{\ell}}(x_i;\lambda), \quad i = 1, \ldots, k-1,\\
&p_k = \alpha \mathrm{D}_\lambda \Phi_{\frac{\Delta s_k T}{\ell}}(x_k;\lambda).
\end{aligned}
$$

We have

$$Jy = b \;\Leftrightarrow\; [G, g, p]\begin{pmatrix} x \\ T \end{pmatrix} = b \;\Leftrightarrow\; Gx = b - gT - p\lambda,$$

so we can use block Gaussian elimination to solve these linear systems. This yields the following algorithm:

1.) Compute the condensed right hand side

$$b_c := C(G, b, k) = b_k + G_k b_{k-1} + \cdots + G_k \cdots G_2 b_1. \tag{2.30}$$

2.) Compute the condensed matrix

$$M_c := [G_c - \mathrm{id}, g_c, p_c] \text{ with } G_c := G_k \cdots G_1, \quad g_c := C(G, g, k), \quad p_c := C(G, p, k). \tag{2.31}$$

3.) Compute a solution of the condensed system

$$M_c \begin{pmatrix} x_1 \\ T \\ \lambda \end{pmatrix} = b_c,$$

for example,

$$\begin{pmatrix} x_1 \\ T \\ \lambda \end{pmatrix} = M_c^+ \, b_c,$$

by QR-decomposition.

4.) Compute x via the explicit recursion

$$x_i = G_{i-1} x_{i-1} - b_{i-1} + g_{i-1} T + p_{i-1} \lambda \quad \text{for} \quad i = 2, \ldots, k. \tag{2.32}$$

We have now obtained a solution $y = J^- b$ where J^- is an outer inverse of J. To compute the solution $J^+ b$ where J^+ is the Moore-Penrose pseudo-inverse of J we have to add one more step:

5.) Compute the kernel of J. Let $t = (t_x, t_T, t_\lambda)$ be a kernel vector where $t_x = (t_1, t_2, \ldots, t_k)$. Starting from a tangent of the condensed system which satisfies

$$[G_c - \mathrm{id}, g_c, p_c] \begin{pmatrix} t_1 \\ t_T \\ t_\lambda \end{pmatrix} = 0,$$

we obtain a tangent t of the whole system by

$$t_i = G_{i-1} t_{i-1} + g_{i-1} t_T + p_{i-1} t_\lambda \quad \text{for} \quad i = 2, \ldots, k,$$

and normalization.
Assume that J has full rank and let $t^{(1)}, \ldots t^{(q+1)}$ be an orthonormal basis of $\ker(J)$. Then we project $y \to y - \sum_{i=1}^{q+1} \langle t^{(i)}, y \rangle t^{(i)}$.

An easy computation shows that in a solution point $\bar{y} = (\bar{x}, \bar{T}, 0)$ we have

$$[G_c - \mathrm{id}, g_c, p_c] = [\alpha \mathrm{D}_x \Phi_{\frac{\bar{T}}{\ell}}(\bar{x}_1) - \mathrm{id}, \frac{1}{\ell} f_H(\bar{x}_1), \mathrm{D}_\lambda \Phi_{\frac{\bar{T}}{\ell}}(\bar{x}_1; \lambda = 0)], \tag{2.33}$$

so the condensed matrix $M_c = [G_c - \mathrm{id}, g_c, p_c]$ equals the Jacobian (2.23) of the single shooting approach (2.22) in the first multiple shooting point $\bar{x}_1$. The Jacobian J is regular iff M_c is regular. Therefore we get the following proposition, analogously to the single shooting case (Theorem 2.5):

Proposition 2.12 *The Jacobian J from (2.29) of the multiple shooting method (2.27) applied to the differential equation (2.20) is regular at a periodic orbit of the Hamiltonian system (2.1) if the periodic orbit is non-degenerate in the sense of Definition 2.3. In this case the Gauss-Newton method (2.17) applied to (2.27) converges for sufficiently good initial data.*

Remark 2.13 In the numerical implementation of the block Gaussian elimination *iterative refinement sweeps* have to be used to stabilize this numerical method, cf. [11, Section 7.1.1], [12, Section 8] and the references therein. Standard refinement methods only converge if $\epsilon k(2n + k)\kappa[0, T/\ell] \ll 1$ where $\kappa[t_0, t]$ is the condition number for the initial value problem for any interval $[t_0, t]$ and ϵ is the machine precision. However, $\kappa[0, T/\ell]$ is the condition number corresponding to the single shooting method! In contrast, the method of iterative refinement sweeps converges if it can be started (which is usually possible in realistic applications, cf [12]) and if the much weaker condition $\epsilon k(2n+k) \max_{j=1,\ldots,k} \kappa[t_j, t_{j+1}] \ll 1$ is satisfied. Here $\{t_j = s_j T/\ell,\ \ j = 1, \ldots k\}$ is the multiple-shooting time grid. Note that the stronger condition $\mathrm{TOL} * \max_{j=1,\ldots,k} \kappa[t_j, t_{j+1}] \ll \mathrm{eps}$ for the tolerance TOL of the initial value problem solvers in terms of the user prescribed accuracy eps has to be satisfied in the multiple shooting method anyway.

Continuation tangent for energy parametrization As continuation tangent for the branch of periodic orbits parametrized by energy we take the kernel vector t^E of J which is orthogonal to $t^f = (t^f_x, 0, 0)$ where $t^f_x = (t^f_1, \ldots t^f_k)$ and $t^f_i = f_H(\bar{x}_i)$, $i = 1, \ldots k$.

2.3.5 Fixing the energy in the multiple shooting ansatz

In this case the equation

$$F^E(x_1, \ldots, x_k, T, \lambda) = 0 \tag{2.34}$$

maps from $X^k \times \mathbb{R}^2 \subseteq \mathbb{R}^{nk+2} \to \mathbb{R}^{nk+1}$, we have $F^E = (F_1, \ldots, F_k, F_E)$ where F_i is as in (2.28), $i = 1, \ldots, k$, and we choose F_E as an average of the Hamiltonian over the multiple shooting points of the periodic orbit:

$$F_E(x_1, \ldots, x_k, T, \lambda) = \frac{1}{k} \sum_{i=1}^{k} H(x_i) - E.$$

Another row has to be added to the derivative $\mathrm{D}F(x, T, \lambda)$ of F from (2.29):

$$J = \mathrm{D}F^E(x, T, \lambda) = \begin{pmatrix} G & g & p \\ l & 0 & 0 \end{pmatrix}, \tag{2.35}$$

where

$$l_i = \frac{1}{k} \mathrm{D}H(x_i), \quad i = 1, \ldots, k.$$

Let $b = (b_x, b_l) \in \mathbb{R}^{kn} \times \mathbb{R}$. Then we have

$$Jy = b \ \Leftrightarrow \ \begin{pmatrix} G & g & p \\ l & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ T \\ \lambda \end{pmatrix} = \begin{pmatrix} b_x \\ b_l \end{pmatrix} \ \Leftrightarrow \ Gx = b_x - gT - p\lambda, \quad lx = b_l. \tag{2.36}$$

We call b_l the constraint right hand side. We can solve (2.36) by adding the following steps to the block Gaussian elimination from Section 2.3.4:

1.) In step 1 we compute the condensed right hand side $b_c = (b_{c,x}, b_{c,l})$: this involves computing the condensed right hand side $b_{c,x} = C(G, b, k)$, cf. (2.30), and the condensed constraint right hand side $b_{c,l}$. The latter is defined as $b_{c,l} = CS(G, b, b_l, k)$ with

$$\begin{aligned} CS(G, b, b_l, k) = &= b_l + l_2 b_1 + \ldots + l_k(b_{k-1} + \ldots G_{k-1} \ldots G_2 b_1) \\ &= b_l + \sum_{i=2}^{k} l_i C(G, b, i-1). \end{aligned}$$

2.) In step 2 we also compute the condensed matrix

$$M_c^E = \begin{pmatrix} G_c & g_c & p_c \\ l_c^G & l_c^g & l_c^p \end{pmatrix} \tag{2.37}$$

where G_c, g_c and p_c are as in (2.31) and the condensed constraint matrices l_c^G, l_c^g, l_c^p are given by

$$l_c^G = l_k G_{k-1} \cdot \ldots \cdot G_1 + \ldots + l_2 G_1 + l_1, \quad l_c^g = CS(G, g, 0, k), \quad l_c^p = CS(G, p, 0, k). \tag{2.38}$$

The rest is now analogous to Section 2.3.4.

Derivation of the modified block Gaussian elimination

The solution of the recursion (2.32) is

$$x_i = G_{i-1} \cdot \ldots \cdot G_1 x_1 + C(G, Tg + \lambda p - b, i-1), \quad i = 2, \ldots, k.$$

Inserting this into the linear constraint equation $lx = b_l$ we get

$$\sum_{i=1}^{k} l_i (G_{i-1} \cdot \ldots \cdot G_1 x_1 + C(G, Tg + \lambda p - b, i-1)) = b_l$$

which is equivalent to

$$l_c^G x_1 + T l_c^g + \lambda l_c^p = b_{c,l}.$$

Proposition 2.14 *If the periodic orbit through $\bar{x}$ with energy $\bar{E} = H(\bar{x})$ is non-degenerate then the Gauss-Newton method (2.17) applied to (2.34) converges for good enough initial data and energies $E \approx \bar{E}$.*

Proof. It suffices to show that the condensed matrix M_c^E from (2.37) has full rank. By the non-degeneracy assumption and (2.33) the kernel of $M_c = [G_c - \mathrm{id}, g_c, p_c]$ is two-dimensional and spanned by the vectors $t_c^E = (t_1^E, t_T^E, 0)$ and $t_c^f = (f(\bar{x}_1), 0, 0)$ where $\mathrm{D}H(\bar{x}_1) t_1^E \neq 0$. We show that t_c^E is not a kernel vector of M_c^E which implies that M_c^E has a one-dimensional kernel and therefore full rank. First we show that $l_c^g = 0$ in the periodic orbit. Since $C(G, g, i-1) = \frac{s_i}{\ell} f(\bar{x}_i)$ in the solution and $l_i = \frac{1}{k} \mathrm{D}H(\bar{x}_i)$ we have $l_i C(G, g, i-1) = 0$ and thus $l_c^g = 0$. As a consequence we need to show that $l_c^G t_1^E \neq 0$. From (2.38) we conclude that in a periodic orbit

$$l_c^G = \frac{1}{k} \left(\mathrm{D}H(\bar{x}_k) \mathrm{D}\Phi_{s_k \bar{T}/\ell}(\bar{x}_1) + \ldots + \mathrm{D}H(\bar{x}_2) \mathrm{D}\Phi_{s_2 \bar{T}/\ell}(\bar{x}_1) + \mathrm{D}H(\bar{x}_1) \right).$$

Now the fact that $\bar{x}_i = \Phi_{s_i \bar{T}/\ell}(x_1)$, $i = 1, 2, \ldots, k$, and (2.5) imply that $l_c^G = \mathrm{D}H(\bar{x}_1)$. Hence we have $l_c^G t_1^E \neq 0$ and M_c^E has full rank.

■

Remark 2.15 This method easily extends to the case of several constraint equations and we use it to compute relative periodic orbits with fixed energy and/or momentum in the next section.

3 Numerical continuation of relative periodic orbits

Now we assume that the Hamiltonian system (2.1) has a *continuous* symmetry group $\Gamma \subseteq \mathrm{SP}(n)$. We moreover assume that Γ is a compact group, i.e., after a coordinate transformation of $\mathbb{R}^n$ it becomes a subset of $\mathrm{O}(n)$. Such continuous matrix groups are examples of *Lie groups* [2, 26]. The easiest example of a Lie group is the group of rotations and reflections in the plane, $\mathrm{O}(2)$, or in three-dimensional space, $\mathrm{O}(3)$, and we will encounter these groups in the numerical continuation of periodic orbits of N-body problems, see Section 4.3 below.

3.1 Momentum maps

We first review the definition of momentum maps. The tangent space $\mathbf{g} = T_{\mathrm{id}}\Gamma$ of Γ at $\gamma = \mathrm{id}$ is called the Lie algebra of Γ. Its elements ξ are called *infinitesimal symmetries*. By Noether's theorem locally there is a conserved quantity $\mathbf{J}_\xi$ of (2.1) for each $\xi \in \mathbf{g}$ such that $\mathbf{J}_\xi$ is the Hamiltonian for the flow $x \to \exp(t\xi)x$ [1, 26]. Moreover $\mathbf{J}_\xi$ is linear in ξ, so that $\mathbf{J}$ maps to the dual $\mathbf{g}^*$ of the Lie algebra $\mathbf{g}$ of Γ. We assume that $\mathbf{J}$ is defined on the whole of $\mathbb{R}^n$. The function $\mathbf{J} : \mathbb{R}^n \to \mathbf{g}^*$ is then called the *momentum* map of the symmetry group Γ.

Example 3.1 In the case of rotational symmetries $\Gamma = \mathrm{SO}(3)$ the space of momenta is $\mathbf{g}^* = \mathrm{so}(3)^* \equiv \mathbb{R}^3$ and $\mathbf{J} : \mathbb{R}^n \to \mathbb{R}^3$ is the angular momentum, see Section 4 below for an example from celestial mechanics.

These additional conserved quantities imply a higher degeneracy of periodic orbits and hence a higher multiplicity of the eigenvalue 1 of the derivative of the Poincaré map. Therefore they have to be taken into account when designing numerical continuation schemes for periodic orbits.

For later reference we now describe the symmetry properties of the momentum map. By

$$\gamma\mathbf{J}(x) := \mathbf{J}(\gamma x), \quad x \in \mathbb{R}^n, \quad \gamma \in \Gamma, \tag{3.1}$$

a group action is defined on the space of momenta $\mathbf{g}^*$ such that the momentum map $\mathbf{J}$ commutes with the group action, i.e., it is Γ-equivariant [26]. We assume in the following that this group action on $\mathbf{g}^*$ is the *coadjoint action* of Γ on $\mathbf{g}^*$ which is defined below.

Definition 3.2 *The* adjoint action *of* Γ *on* $\mathbf{g}$ *is defined by*

$$\mathrm{Ad}_\gamma \xi = \gamma\xi\gamma^{-1}, \quad \gamma \in \Gamma, \xi \in \mathbf{g},$$

and the coadjoint action by

$$\gamma\mu := (\mathrm{Ad}^*_\gamma)^{-1}\mu, \quad \gamma \in \Gamma, \mu \in \mathbf{g}^*, \tag{3.2}$$

where

$$(\mathrm{Ad}^*_\gamma\mu)(\xi) = \mu(\mathrm{Ad}_\gamma\xi), \quad \gamma \in \Gamma, \quad \xi \in \mathbf{g}, \quad \mu \in \mathbf{g}^*.$$

The corresponding infinitesimal adjoint and coadjoint group actions *are given by*

$$\mathrm{ad}_\xi\eta := [\xi, \eta] := \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ad}_{\exp(t\xi)}\eta|_{t=0}, \quad \xi, \eta \in \mathbf{g},$$

and

$$\xi\mu := -\mathrm{ad}^*_\xi\mu \quad \textit{where} \quad (\mathrm{ad}^*_\xi\mu)(\eta) = \mu(\mathrm{ad}_\xi\eta), \quad \xi, \eta \in \mathbf{g}, \mu \in \mathbf{g}^*. \tag{3.3}$$

Note that $[\xi,\eta]$ is the Lie bracket on the Lie algebra $\mathbf{g}$ and for matrix groups, as considered here, it is the commutator of the matrices ξ and η: $[\xi,\eta]=\xi\eta-\eta\xi$.

Example 3.3 In the case of rotational symmetry where $\mathbf{g}=\mathrm{so}(3)\simeq\mathbb{R}^3$ the adjoint and coadjoint actions are just the usual multiplication by matrices in SO(3). Here the identification $\mathrm{so}(3)\simeq\mathbb{R}^3$ is given by the map

$$\xi=(\xi_1,\xi_2,\xi_3)\to\begin{pmatrix}0&\xi_3&-\xi_2\\-\xi_3&0&\xi_1\\\xi_2&-\xi_1&0\end{pmatrix}. \tag{3.4}$$

The Lie bracket becomes $[\xi,\eta]=\xi\times\eta$, where $\xi,\eta\in\mathbb{R}^3\simeq\mathrm{so}(3)$.

Note that from (3.1) and (3.2) we get

$$\mathbf{J}(\gamma x)=(\mathrm{Ad}^*_\gamma)^{-1}\mathbf{J}(x)\quad\text{ for all }\quad\gamma\in\Gamma,\quad x\in\mathbb{R}^n,$$

and therefore

$$\mathbf{J}_\xi(\gamma x)=\mathbf{J}_{\mathrm{Ad}^{-1}_\gamma\xi}(x),\quad\gamma\in\Gamma. \tag{3.5}$$

Since the symmetry group is assumed to be compact the momentum map $\mathbf{J}$ can always be chosen to be equivariant with respect to the *coadjoint action* of Γ on $\mathbf{g}^*$ by averaging. Moreover, the adjoint action is by orthogonal matrices and so adjoint and coadjoint action coincide, see [26].

3.2 Relative periodic orbits

In systems with continuous symmetries *relative periodic orbits* are ubiquitous. These are orbits which are periodic after symmetry reduction, but in general are not periodic orbits for the original system:

Definition 3.4 *A point $\bar{x}$ lies on a relative periodic orbit (RPO) $\bar{\mathcal{P}}$ if there exists $\tau>0$ such that $\Phi_\tau(\bar{x})\in\Gamma\bar{x}$. The infimum $\bar{\tau}$ of such τ is called the* relative period *of the relative periodic orbit and the element $\bar{\sigma}\in\Gamma$ such that $\bar{\sigma}\Phi_{\bar{\tau}}(\bar{x})=\bar{x}$ is called a* phase-shift symmetry *or* drift symmetry *of the relative periodic orbit. The relative periodic orbit $\bar{\mathcal{P}}$ itself is given by*

$$\bar{\mathcal{P}}=\{\gamma\Phi_t(\bar{x});\quad t\in\mathbb{R},\gamma\in\Gamma\}.$$

As in the previous section, we assume the isotropy K of the point $\bar{x}$ of the relative periodic orbit to be trivial, unless stated otherwise.

If $\bar{\tau}=0$ so that $\Phi_t(\bar{x})\in\Gamma\bar{x}$ for all $t\in\mathbb{R}$ then $\bar{x}$ lies on a *relative equilibrium*, i.e., it is an equilibrium in the space of group orbits. A $\bar{T}$-periodic orbit with drift symmetry α of order ℓ is an RPO with relative period $\bar{\tau}=\bar{T}/\ell$.

3.2.1 Drift-momentum pairs and drift velocities of RPOs

The momentum $\bar{\mu}$ and drift symmetry $\bar{\sigma}$ of a relative periodic orbit satisfy the following relationship which is essential for studying the persistence of the relative periodic orbit to nearby momentum level sets (see Section 3.5):

Lemma 3.5 *Let $\bar{x}$ lie on a relative periodic orbit with drift symmetry $\bar{\sigma}$ and momentum $\bar{\mu}=\mathbf{J}(\bar{x})$ at $\bar{x}$. Then*

$$\bar{\sigma}\bar{\mu}=\bar{\mu}, \tag{3.6}$$

where the action of Γ on $\mathbf{g}^*$ is as in (3.2).

Proof. Let, as before, $\bar{\tau}$ be the relative period of the RPO. The lemma then simply follows from the fact that $\mathbf{J}$ is preserved by the flow, and so

$$\bar{\sigma}\bar{\mu} = \bar{\sigma}\mathbf{J}(\bar{x}) = \mathbf{J}(\bar{\sigma}\bar{x}) = \mathbf{J}(\Phi_{-\bar{\tau}}(\bar{x})) = \mathbf{J}(\bar{x}) = \bar{\mu}.$$

■

Definition 3.6 *[34] We call pairs* $(\sigma, \mu) \in \Gamma \times \mathbf{g}^*$ *satisfying* (3.6) drift-momentum pairs *and denote the space of drift-momentum pairs by*

$$(\Gamma \times \mathbf{g}^*)^c := \{(\gamma, \mu) \in \Gamma \times \mathbf{g}^*, \quad \gamma\mu = \mu\}. \tag{3.7}$$

Example 3.7 In the case $\Gamma = \mathrm{SO}(3)$, see Example 3.1 and 3.3, a drift-momentum pair (σ, μ) consists of an angular momentum vector $\mu \in \mathbb{R}^3 \simeq \mathrm{so}(3)^*$ together with a rotation $\sigma \in \mathrm{SO}(3)$ around this vector.

For later reference we define the notion of isotropy subalgebras of drift symmetries $\sigma \in \Gamma$, momenta $\mu \in \mathbf{g}^*$ and drift-momentum pairs $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$.

Definition 3.8

(i) Let

$$\mathbf{g}_\sigma = \{\xi \in \mathbf{g}, \exp(t\xi)\sigma\exp(-t\xi) = \sigma \text{ for all } t \in \mathbb{R}\} = \{\xi \in \mathbf{g}, \quad \mathrm{Ad}_{\bar{\sigma}}\xi = \xi\} = \mathrm{Fix}_{\mathbf{g}}(\sigma)$$

be the isotropy subalgebra *of* $\sigma \in \Gamma$ *or, equivalently, the fixed point space of* σ *in* $\mathbf{g}$. *Moreover let* $r_\sigma = \dim \mathbf{g}_\sigma$.

(ii) Let

$$\mathbf{g}_\mu = \{\xi \in \mathbf{g}, \exp(t\xi)\mu = \mu \text{ for all } t \in \mathbb{R}\} = \{\xi \in \mathbf{g}, \quad \xi\mu = 0\}$$

be the isotropy subalgebra *of the momentum* $\mu \in \mathbf{g}^*$ *with respect to the coadjoint action (3.2) and the infinitesimal coadjoint action (3.3), and let* $r_\mu = \dim \mathbf{g}_\mu$.

(iii) Let

$$\mathbf{g}_{(\sigma,\mu)} = \{\xi \in \mathbf{g}, \exp(t\xi)\mu = \mu, \exp(t\xi)\sigma\exp(-t\xi) = \sigma \text{ for all } t \in \mathbb{R}\} = \mathrm{Fix}_{\mathbf{g}_\mu}(\sigma)$$

be the isotropy subalgebra *of the drift-momentum pair* $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$ *and let* $r_{(\sigma,\mu)} = \dim \mathbf{g}_{(\sigma,\mu)}$.

Let

$$Z(\sigma) := \Gamma_\sigma = \{\gamma \in \Gamma, \quad \gamma\sigma\gamma^{-1} = \sigma\} \quad \text{and} \quad Z(\xi) := \Gamma_\xi = \{\gamma \in \Gamma, \quad \mathrm{Ad}_\gamma\xi = \xi\} \tag{3.8}$$

denote the centralizers of $\sigma \in \Gamma$ and $\xi \in \mathbf{g}$ and let

$$\Gamma_\mu = \{\gamma \in \Gamma, \ \gamma\mu = \mu\} \tag{3.9}$$

be the isotropy group of μ with respect to the coadjoint action (3.2). Note that with this notation $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$ if and only if $\sigma \in \Gamma_\mu$. Finally let

$$\Gamma_{(\sigma,\mu)} = \Gamma_\sigma \cap \Gamma_\mu \tag{3.10}$$

be the isotropy subgroup of the drift-momentum pair $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$.

The next lemma shows that relative periodic orbits of compact group actions are periodic orbits in a comoving frame:

Lemma 3.9

a) Any element σ of a compact group Γ can be decomposed as

$$\sigma = \alpha \exp(-\xi),$$

for some $\xi \in \mathbf{g}$ and $\alpha \in \Gamma$ such that

$$\alpha^\ell = \mathrm{id} \quad \textit{for some } \ell \in \mathbb{N}, \quad \mathrm{Ad}_\alpha \xi = \xi,$$

and such that

$$Z(\sigma) = Z(\alpha) \cap Z(\xi).$$

b) For any relative periodic orbit with drift-momentum pair $(\bar\sigma, \bar\mu) \in (\Gamma \times \mathbf{g}^*)^c$, trivial isotropy K and relative period $\bar\tau$ there is a frame moving with velocity $\bar\xi \in \mathbf{g}_{(\bar\sigma,\bar\mu)}$, called drift velocity *of the RPO with respect to $\bar x$, and some integer ℓ such that in this comoving frame the RPO becomes a periodic orbit of period $\bar T = \ell\bar\tau$ and drift symmetry $\alpha \in \Gamma_{\bar\mu}$. Moreover $\bar\sigma = \alpha \exp(-\bar\tau\bar\xi)$.*

Proof.

a) Let C be the group generated by σ. The group C is abelian and therefore of the form $C = \mathbb{Z}_\ell \times \mathbb{T}^m$ for some $\ell, m \in \mathbb{N}$. Here $\mathbb{T}^m$ denotes an m-dimensional torus. We choose α to be the generator of $\mathbb{Z}_\ell$ which satifies $\sigma \in \alpha\mathbb{T}^m$ and choose ξ in the Lie algebra of $\mathbb{T}^m$ such that $\sigma = \alpha\exp(-\xi)$. If then $\gamma \in Z(\sigma)$ then

$$\gamma \in Z(C) := \bigcap_{\gamma_C \in C} Z(\gamma_C)$$

and so in particular $\gamma \in Z(\alpha) \cap Z(\xi)$.

b) By Lemma 3.5 we have $\bar\sigma \in \Gamma_{\bar\mu}$. From a), with Γ replaced by $\Gamma_{\bar\mu}$, we know that we can decompose $\bar\sigma = \alpha\exp(-\xi)$ where $\alpha \in \Gamma_\mu$ and $\xi \in \mathbf{g}_{\bar\mu}$ such that α and ξ commute. Hence ξ and $\bar\sigma$ commute and so $\xi \in \mathbf{g}_{(\bar\sigma,\bar\mu)}$. Let $\bar\xi = \frac{1}{\bar\tau}\xi$. Then $\bar x$ lies on a $\bar T$-periodic orbit in a system moving with velocity $\bar\xi$.

■

Remarks 3.10

a) Note that the decomposition $\sigma = \alpha\exp(-\xi)$ in Lemma 3.9 is in general not unique: for example, assume that the group C generated by σ is continuous. Let η be an infinitesimal rotation in the Lie algebra of C which generates the rotation group $\exp(\phi\eta) = R_\phi \in C$, $\phi \in [0, 2\pi]$. Then other possible choices for α and ξ would be $\bar\alpha = R_{2\pi j/\ell}\alpha$ where $j \in \mathbb{Z}$, $\gcd(\ell, j) = 1$, and $\bar\xi = \xi + 2\pi(n + \frac{j}{\ell})\eta$, $n \in \mathbb{N}$.

b) If the spatial symmetry group K of the RPO is not trivial then we can restrict the dynamics to $\mathrm{Fix}(K)$, see Remark 2.2, and replace the symmetry group by $N(K)/K$. The identity component $N(K)^{\mathrm{id}}$ of $N(K)$ satisfies $N(K)^{\mathrm{id}} = Z(K)^{\mathrm{id}}K^{\mathrm{id}}$ where $Z(K)$ denotes the centralizer of K, see e.g. [36] and references therein. It is therefore possible to choose a representative for the drift velocity $\bar\xi$ of the RPO in $\mathbf{g}$ such that $\bar\xi$ lies in the Lie algebra of $Z(K)$; however, α can in general not be chosen to commute with K, see [36].

3.2.2 Linearization along non-degenerate RPOs

Let $\bar{x}$ lie on an RPO $\bar{\mathcal{P}}$ with relative period $\bar{\tau}$. We assume without loss of generality that the isotropy K of the relative periodic orbit is finite (if not, we restrict the dynamics to $\mathrm{Fix}(K)$ so that K is trivial, cf. Remark 2.2). We call a section $S := S_{\bar{x}}$ which is transverse to the RPO at $\bar{x}$, i.e., transverse to $\mathbf{g}\bar{x} \oplus \mathrm{span}(f_H(\bar{x}))$, a Poincaré section at $\bar{x}$. We define the reduced Poincaré map $\Pi_{\mathrm{red}} : S \to S$ analogously to the case of discrete symmetry groups (2.13) as follows (see [36, 34]). For $x \in S$ close to $\bar{x}$ there are unique $\gamma(x) \in \Gamma$, $\gamma(x) \approx \bar{\sigma}$, and $\tau(x) \approx \bar{\tau}$ such that $\gamma(x)\Phi_{\tau(x)}(x) \in S$ (this follows from the implicit function theorem since we assume that the isotropy K of the RPO is finite). Now define $\Pi_{\mathrm{red}}(x) = \gamma(x)\Phi_{\tau(x)}(x)$.

Definition 3.11 *A relative periodic orbit of a Hamiltonian system (2.1) on the open set $X \subseteq \mathbb{R}^n$ with continuous symmetry group Γ is called* non-degenerate*, if it is not a relative equilibrium and if $\Pi_{\mathrm{red}}^{\bar{E},\bar{\mu}} : S^{\bar{E},\bar{\mu}} \to S^{\bar{E},\bar{\mu}}$ does not have an eigenvalue 1 at a point $\bar{x}$ of the relative periodic orbit. Here $\bar{E} = H(\bar{x})$ and $\bar{\mu} = \mathbf{J}(\bar{x})$ are the energy and momentum of $\bar{x}$, and $S^{\bar{E},\bar{\mu}}$ is a Poincaré section transverse to the relative periodic orbit at $\bar{x}$ inside the energy-momentum level set*

$$X^{\bar{E},\bar{\mu}} = \{x \in X, \quad H(x) = \bar{E}, \ \mathbf{J}(x) = \bar{\mu}\}$$

of $\bar{x}$.

Let $\bar{x}$ lie on an RPO. Then $\bar{x}$ is a fixed point of $\bar{\sigma}\Phi_{\bar{\tau}}(\bar{x}) = \bar{x}$. If the RPO is non-degenerate then the eigenspace of the derivative $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ of the fixed point equation $\bar{\sigma}\Phi_{\bar{\tau}}(\bar{x}) = \bar{x}$ to the eigenvalue 1 has the lowest possible dimension as the following proposition shows:

Proposition 3.12 *Let $\bar{x}$ lie on an RPO of (2.1) with drift symmetry $\bar{\sigma}$ and momentum $\bar{\mu} = \mathbf{J}(\bar{x})$. Then the following holds true:*

a) As for Hamiltonian systems with discrete symmetries, cf. (2.19) and (2.15), we have

$$\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})f_H(\bar{x}) = f_H(\bar{x}), \quad \mathrm{D}H(\bar{x})\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x}) = \mathrm{D}H(\bar{x}).$$

b) Moreover,

$$\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})\eta\bar{x} = (\mathrm{Ad}_{\bar{\sigma}}\eta)\bar{x}, \quad \eta \in \mathbf{g}, \tag{3.11}$$

and

$$\mathrm{D}\mathbf{J}_{\eta}(\bar{x})\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x}) = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar{\sigma}}^{-1}\eta}(\bar{x}). \tag{3.12}$$

c) Let $\bar{x}$ lie on a proper RPO (i.e., not a relative equilibrium) and let the isotropy K of $\bar{x}$ be finite. Then the following holds true:

(i) The geometric multiplicity of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to the eigenvalue 1 is at least $1 + r_{\bar{\sigma}}$.

(ii) The generalized eigenspace of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to the eigenvalue 1 has at least dimension $2 + r_{\bar{\sigma}} + r_{(\bar{\sigma},\bar{\mu})}$ and exactly this dimension if the RPO is non-degenerate.

Proof. Most of this proposition is implicitly contained in [37, Sect. 6.2, 6.3]. For sake of completeness we include the proof:

a) The first relation follows from differentiating the relation $\bar{\sigma}\Phi_{\bar{\tau}}(\Phi_t(\bar{x})) = \Phi_t(\bar{x})$ with respect to t at $t = 0$. The second equation can be proved like (2.15) with α replaced by $\bar{\sigma}$.

b) By equivariance of $\Phi_{\bar{\tau}}(\cdot)$ we have $\eta\Phi_{\bar{\tau}}(\bar{x}) = \mathrm{D}\Phi_{\bar{\tau}}(\bar{x})\eta\bar{x}$ for $\eta \in \mathbf{g}$ and so

$$\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})\eta\bar{x} = \bar{\sigma}\eta\Phi_{\bar{\tau}}(\bar{x}) = \bar{\sigma}\eta\bar{\sigma}^{-1}\bar{x} = (\mathrm{Ad}_{\bar{\sigma}}\eta)\bar{x}.$$

From (3.5) we get

$$\mathrm{D}\mathbf{J}_\eta(\bar\sigma x)\bar\sigma = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar\sigma}^{-1}\eta}(x),$$

and so, with $x = \bar\sigma^{-1}\bar x$,

$$\mathrm{D}\mathbf{J}_\eta(\bar x)\bar\sigma = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar\sigma}^{-1}\eta}(\bar\sigma^{-1}\bar x).$$

Momentum conservation, i.e., $\mathbf{J}(x) = \mathbf{J}(\Phi_t(x))$ for all t, x, implies

$$\mathrm{D}\mathbf{J}(x) = \mathrm{D}\mathbf{J}(\Phi_t(x))\mathrm{D}\Phi_t(x).$$

Hence

$$\mathrm{D}\mathbf{J}_\eta(\bar x)\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x) = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar\sigma}^{-1}\eta}(\bar\sigma^{-1}\bar x)\mathrm{D}\Phi_{\bar\tau}(\bar x) = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar\sigma}^{-1}\eta}(\Phi_{\bar\tau}(\bar x))\mathrm{D}\Phi_{\bar\tau}(\bar x) = \mathrm{D}\mathbf{J}_{\mathrm{Ad}_{\bar\sigma}^{-1}\eta}(\bar x).$$

c) (i) From (3.11) and the fact that $\xi\bar x \neq 0$ for $\xi \in \mathbf{g}$, $\xi \neq 0$ (as K is finite) we see that the set $\{\xi\bar x,\ \ \xi \in \mathrm{Fix}_{\mathbf{g}}(\bar\sigma)\}$ is a $\dim(\mathrm{Fix}_{\mathbf{g}}(\bar\sigma))$-dimensional subset of the eigenspace of $\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x)$ to the eigenvalue 1. By part a), $f_H(\bar x)$ is an eigenvector to the eigenvalue 1 as well. Let $\xi_1, \ldots, \xi_s$, $s = r_{\bar\sigma} = \dim \mathrm{Fix}_{\mathbf{g}}(\bar\sigma)$, be a basis of $\mathrm{Fix}_{\mathbf{g}}(\bar\sigma)$. Then the vectors $f_H(\bar x)$ and $\xi_i\bar x$, $i = 1, \ldots, s$, are linearly independent, otherwise $\bar x$ would lie on a relative equilibrium. Therefore the geometric multiplicity of the eigenvalue 1 of $\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x)$ is at least $r_{\bar\sigma} + 1$. This proves (i).

(ii) By (3.12) the row vectors $\mathrm{D}\mathbf{J}_\xi(\bar x)$, $\xi \in \mathrm{Fix}_{\mathbf{g}}(\bar\sigma) = \mathbf{g}_{\bar\sigma}$, are left eigenvectors of $\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x)$ to the eigenvalue 1. To compute the algebraic multiplicity of the eigenvalue 1 of $\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x)$ we need to determine the dimension of the vector space formed by those left eigenvectors $\mathrm{D}\mathbf{J}_\xi(\bar x)$ which annihilate the right eigenvectors $\{\eta\bar x,\ \eta \in \mathrm{Fix}_{\mathbf{g}}(\bar\sigma)\}$. Using (3.5) we compute that for $\xi, \eta \in \mathbf{g}$

$$\begin{aligned}\mathrm{D}\mathbf{J}_\xi(\bar x)\eta\bar x &= \frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{J}_\xi(\exp(\tau\eta)\bar x)|_{\tau=0} = \mathbf{J}_{\frac{\mathrm{d}}{\mathrm{d}\tau}\mathrm{Ad}_{\exp(-\tau\eta)}\xi|_{\tau=0}}(\bar x) = \mathbf{J}_{-\mathrm{ad}_\eta\xi}(\bar x)\\ &= \bar\mu(\mathrm{ad}_\xi\eta) = \mathrm{ad}^*_\xi\bar\mu(\eta).\end{aligned}$$

Hence, $\mathrm{D}\mathbf{J}_\xi(\bar x)$ annihilates the eigenvectors $\eta\bar x$, $\eta \in \mathrm{Fix}_{\mathbf{g}}(\bar\sigma)$, if and only if

$$\mathrm{ad}^*_\xi\bar\mu|_{\mathrm{Fix}_{\mathbf{g}}(\bar\sigma)} = 0. \tag{3.13}$$

Note that $(\mathrm{id}-\mathrm{Ad}_{\bar\sigma})\mathbf{g}$ is transverse $\mathrm{Fix}_{\mathbf{g}}(\bar\sigma)$, i.e., $(\mathrm{id}-\mathrm{Ad}_{\bar\sigma})\mathbf{g}\oplus\mathrm{Fix}_{\mathbf{g}}(\bar\sigma) = \mathbf{g}$. Moreover, for $\eta \in \mathbf{g}$, $\xi \in \mathrm{Fix}_{\mathbf{g}}(\bar\sigma)$ we get

$$\begin{aligned}\mathrm{ad}^*_\xi\bar\mu((\mathrm{id}-\mathrm{Ad}_{\bar\sigma})\eta) &= \bar\mu(\mathrm{ad}_\xi((\mathrm{id}-\mathrm{Ad}_{\bar\sigma})\eta)) = \bar\mu(\mathrm{ad}_\xi\eta) - \bar\mu(\mathrm{ad}_\xi\mathrm{Ad}_{\bar\sigma}\eta)\\ &= \bar\mu(\mathrm{ad}_\xi\eta) - \mu(\mathrm{Ad}_{\bar\sigma}\mathrm{ad}_{\mathrm{Ad}_{\bar\sigma}^{-1}\xi}\eta) = \bar\mu(\mathrm{ad}_\xi\eta) - \bar\mu(\mathrm{Ad}_{\bar\sigma}\mathrm{ad}_\xi\eta)\\ &= \bar\mu(\mathrm{ad}_\xi\eta) - \mathrm{Ad}^*_{\bar\sigma}\bar\mu(\mathrm{ad}_\xi\eta) = \bar\mu(\mathrm{ad}_\xi\eta) - \bar\mu(\mathrm{ad}_\xi\eta) = 0.\end{aligned}$$

Here we used that

$$\begin{aligned}\mathrm{ad}_\chi\mathrm{Ad}_\gamma\eta &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\exp(t\chi)\gamma\eta\gamma^{-1}\exp(-t\chi)|_{t=0}\right)|_{t=0}\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\gamma(\gamma^{-1}\exp(t\chi)\gamma)\eta(\gamma^{-1}\exp(-t\chi)\gamma)\gamma^{-1})\right)|_{t=0}\\ &= \mathrm{Ad}_\gamma\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ad}_{\exp(t\mathrm{Ad}_\gamma^{-1}\chi)}\eta|_{t=0} = \mathrm{Ad}_\gamma\mathrm{ad}_{\mathrm{Ad}_\gamma^{-1}\chi}\eta,\end{aligned}$$

and (3.6). So we have $\mathrm{ad}^*_\xi\bar\mu|_{(\mathrm{id}-\mathrm{Ad}_{\bar\sigma})\mathbf{g}} = 0$ and therefore, with (3.13), we see that the left eigenvectors $\mathrm{D}\mathbf{J}_\xi(\bar x)$, $\xi \in \mathbf{g}_{\bar\sigma}$, of $\bar\sigma\mathrm{D}\Phi_{\bar\tau}(\bar x)$ to the eigenvalue 1 annihilate

the eigenvectors $\eta\bar{x}$, $\eta \in \mathrm{Fix}_{\mathbf{g}}(\bar{\sigma})$ if and only if $\mathrm{ad}^*_\xi \bar{\mu} \equiv 0$ which is equivalent to $\xi \in \mathbf{g}_{\bar{\mu}}$. Hence the algebraic multiplicity of the eigenvalue 1 of $\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x})$ is at least $\dim \mathrm{Fix}_{\mathbf{g}_{\bar{\mu}}}(\bar{\sigma}) + \dim \mathrm{Fix}_{\mathbf{g}}(\bar{\sigma})$. But due to energy conservation and phase shift symmetry its algebraic multiplicity is higher:
Let $\xi_1, \ldots, \xi_r$, $r = \dim \mathrm{Fix}_{\mathbf{g}_{\bar{\mu}}}(\bar{\sigma}) = r_{(\bar{\sigma},\bar{\mu})}$, span $\mathrm{Fix}_{\mathbf{g}_{\bar{\mu}}}(\bar{\sigma})$. As we saw in part a), also $\mathrm{D}H(\bar{x})$ is a left eigenvector to the eigenvalue 1. Since both momentum $\mathbf{J}(\cdot)$ and energy $H(\cdot)$ are conserved by the flow we have

$$\mathrm{D}\mathbf{J}(\bar{x}) f_H(\bar{x}) = 0, \quad \mathrm{D}H(\bar{x}) f_H(\bar{x}) = 0.$$

Since H is Γ-invariant, also

$$\mathrm{D}H(\bar{x})\xi\bar{x} = 0, \quad \xi \in \mathbf{g}.$$

Moreover, as we saw in (i), the vectors $f_H(\bar{x})$ and $\xi_i\bar{x}$, $i = 1, \ldots, s$, are linearly independent, and the same holds true for the vectors $\mathrm{D}H(\bar{x})$, $\mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})$, $i = 1, \ldots, r$ (otherwise $\bar{x}$ would lie on a relative equilibrium or it would have continuous isotropy K). Therefore there are linear independent vectors t^E, t^{μ_1}, ..., t^{μ_r} in the generalized eigenspace of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to the eigenvalue 1 with

$$\begin{aligned}
&\mathrm{D}H(\bar{x})t^E = 1, && \mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})t^{\mu_j} = \delta_{ij}, \quad i,j = 1,\ldots,r,\\
&\mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})t^E = 0, && \mathrm{D}H(\bar{x})t^{\mu_i} = 0, \quad i = 1,\ldots,r,\\
&t^E, t^{\mu_i} \perp \{\xi\bar{x}, \xi \in \mathbf{g}_{\bar{\sigma}}\}, && t^E, t^{\mu_i} \perp f_H(\bar{x}), \quad i = 1,\ldots,r.
\end{aligned} \tag{3.14}$$

Hence, the algebraic multiplicity of the eigenvalue 1 of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ is at least $2 + r + r_{\bar{\sigma}}$.
If the relative periodic orbit is non-degenerate then there are no (generalized) eigenvectors of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to the eigenvalue 1 in a section $S^{\bar{E},\bar{\mu}}$ transverse to the RPO at $\bar{x}$ inside the energy-momentum level set of $\bar{x}$. Therefore the dimension of the generalized eigenspace of $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to 1 is exactly $2 + r + r_{\bar{\sigma}}$ in this case. This proves (ii).

■

Remark 3.13 Proposition 3.12 c) ii) strengthens a related result of Muñoz-Almaraz et al [29, Proposition 12]. In our notation, they show that the algebraic multiplicity m_a of the eigenvalue 1 of the linearization $\mathrm{D}\Phi_{\bar{T}}(\bar{x})$ at a $\bar{T}$-periodic orbit of a Γ-symmetric Hamiltonian system satisfies $m_a \geq (\dim \Gamma + 1) + (\dim Z + 1)$ where Z is the centre of Γ. Since spatio-temporal symmetries are not considered in [29], we have $\bar{\sigma} = \mathrm{id}$, and so in this case Proposition 3.12 c) ii) implies that $m_a \geq \dim \Gamma + 2 + r_{\bar{\mu}}$ where $\bar{\mu} = \mathbf{J}(\bar{x})$. As the Lie algebra $\mathbf{z}$ of Z is contained in $\mathbf{g}_\mu$ for any $\mu \in \mathbf{g}^*$ we see that $r_{\bar{\mu}} \geq \dim Z$. Note also that our estimate for m_a is sharp for non-degenerate periodic orbits.

3.3 Numerical continuation for one-dimensional symmetry groups

In this section we assume that the symmetry group Γ is one-dimensional. Denote by $\xi \in \mathbf{g}$ the generator of the identity component Γ^{id} of Γ.

Let, as before, $\bar{x}$ lie on a relative periodic orbit with drift velocity $\bar{\xi} \in \mathbf{g}$, relative period $\bar{\tau}$ and phase-shift symmetry α of order ℓ in the frame moving with velocity $\bar{\xi}$. Hence we have $\bar{\sigma}\Phi_{\bar{\tau}}(\bar{x}) = \bar{x}$ where $\bar{\sigma} = \exp(-\bar{\tau}\bar{\xi})\alpha$. By Lemma 3.5, $\bar{\mu} = \bar{\sigma}\bar{\mu}$ where $\bar{\mu} = \mathbf{J}(\bar{x})$ is the momentum of the RPO at $\bar{x}$. Since the group action on $\mathbf{g}^*$ is linear and $\mathbf{g}^*$ is one-dimensional, the fixed

point space $\mathrm{Fix}_{\mathbf{g}^*}(\bar\sigma)$ of $\bar\sigma$ in the space of momenta $\mathbf{g}^*$ is either $\{0\}$ or the whole of $\mathbf{g}^*$. In the second case $\bar\sigma$ also acts trivially on $\mathbf{g}$ and so we have

$$\mathrm{Ad}_\alpha \eta = \eta, \quad \mathrm{Ad}^*_\alpha \mu = \mu, \quad \mathrm{ad}^*_\eta \mu = 0 \ \text{ for all } \eta \in \mathbf{g},\ \mu \in \mathbf{g}^*, \tag{3.15}$$

and therefore also

$$\mathbf{J}(\alpha x) = \mathbf{J}(x), \quad \mathbf{J}(\exp(t\xi)x) = \mathbf{J}(x) \ \text{ for all } \ x \in \mathbb{R}^n,\ t \in \mathbb{R}. \tag{3.16}$$

In the first case we know that $\mathrm{Ad}_{\bar\sigma}\eta = \eta$ implies that $\eta = 0$ so that any relative periodic orbit with drift symmetry $\bar\sigma$ would actually be periodic and we do not have to consider continuous symmetries at all. The reason for this is that by Proposition 3.12 b) the eigenvectors of $\bar\sigma \mathrm{D}\Phi_{\bar\tau}(\bar x)$ to the eigenvalue 1 which are caused by continuous symmetries or momentum conservation correspond to infinitesimal symmetries $\xi \in \mathbf{g}$ with $\mathrm{Ad}_{\bar\sigma}\xi = \xi$. So there are no such eigenvectors in this case. Therefore from now on we assume that (3.16) holds (cf. Theorem 3.17 for the same trick applied to symmetry groups of arbitrary dimension).

Consider, analogously to (2.20), the differential equation

$$\dot x = f(x, \omega, \lambda_E, \lambda_\mu) = f_H(x) + \lambda_E \nabla H(x) + \lambda_\mu \nabla \mathbf{J}(x) - \omega \xi x. \tag{3.17}$$

Note that for $\lambda_\mu = \lambda_E = 0$ the flow $\Phi_t(\cdot;\omega)$ of (3.17) is the flow of (2.1) in a frame moving with velocity $\omega\xi$. More precisely, $\Phi_t(\cdot;\omega)$ is given by

$$\Phi_t(\cdot;\omega) = \exp(-t\omega\xi)\Phi_t(\cdot)$$

where $\Phi_t(\cdot)$ is the flow of (2.1). Let $\bar T = \ell\bar\tau$ be the period of the RPO in the system moving with velocity $\bar\xi = \bar\omega\xi$. Then the relative periodic orbit satisfies $\bar x = \bar\sigma\Phi_{\bar T/\ell}(\bar x)$, and hence

$$\alpha\Phi_{\bar T/\ell}(\bar x;\bar\omega) = \bar x.$$

3.3.1 Single shooting approach

To compute relative periodic orbits numerically we solve the equation

$$F(x, T, \omega, \lambda_E, \lambda_\mu) = \alpha\Phi_{T/\ell}(x;\omega,\lambda_E,\lambda_\mu) - x = 0 \tag{3.18}$$

where $\Phi_t(\cdot,\omega,\lambda_E,\lambda_\mu)$ is the flow of (3.17). Similarly as for Hamiltonian periodic orbits, see Theorem 2.5, we have the following result:

Theorem 3.14 *Let* $\dim\Gamma = 1$ *and let* $\bar x$ *lie on a non-degenerate RPO* $\bar{\mathcal{P}}$ *with trivial isotropy* K*. Then the following holds true:*

a) The RPO persists to any nearby energy and momentum.

b) Denote $y = (x, T, \omega, \lambda_E, \lambda_\mu)$*. The Jacobian* $\mathrm{D}_y F(\bar y)$ *of (3.18) is regular in the solution point* $\bar y = (\bar x, \bar T, \bar\omega, 0, 0)$ *and therefore the Gauss-Newton method (2.17) applied to (3.18) converges for initial data* $\hat y$ *close to* $(\bar{\mathcal{P}}, \bar T, \bar\omega, 0, 0)$*. Furthermore any solution* $y = (x, T, \omega, \lambda_\mu, \lambda_E)$ *of (3.18) close to* $(\bar{\mathcal{P}}, \bar T, \bar\omega, 0, 0)$ *satisfies* $\lambda_E = \lambda_\mu = 0$ *and hence is an RPO of (2.1).*

Proof.

a) Denote by $S = S_{\bar x} = \bar x + (\mathrm{span}(\xi\bar x, f_H(\bar x)))^\perp$ a Poincaré section transverse to $\bar{\mathcal{P}}$ at $\bar x$. Note that $\mathrm{D}H(\bar x) \neq 0$ since $\bar x$ is not an equilibrium and that $\mathrm{D}H(\bar x)|_{\mathrm{span}(\xi\bar x, f_H(\bar x))} = 0$. Hence $\mathrm{D}H(\bar x)|_S \neq 0$. Similarly $\mathrm{D}\mathbf{J}(\bar x) \neq 0$ as we assume that the isotropy of $\bar x$ is trival. Since

$\mathrm{D}\mathbf{J}(\bar{x})|_{\mathrm{span}(\xi\bar{x}, f_H(\bar{x}))} = 0$ we conclude that $\mathrm{D}\mathbf{J}(\bar{x})|_S \neq 0$. Moreover $\mathrm{D}\mathbf{J}(\bar{x})$ and $\mathrm{D}H(\bar{x})$ are linearly independent on $\mathbb{R}^n$ and hence also on S as $\bar{x}$ does not lie on a relative equilibrium. We conclude that the Poincaré sections

$$S^{E,\mu} = S \cap \{x, \quad H(x) = E, \mathbf{J}(x) = \mu\}$$

are codimension 2 submanifolds of S for any $E \approx \bar{E} = H(\bar{x})$, $\mu \approx \bar{\mu} = \mathbf{J}(\bar{x})$. Consequently $\Pi_{\mathrm{red}}^{E,\mu} : S^{E,\mu} \to S^{E,\mu}$ is smoothly parametrized by E and μ and the non-degenerate fixed point $\bar{x}$ of $\Pi_{\mathrm{red}}^{E,\mu}$ for $E = \bar{E}$, $\mu = \bar{\mu}$ persists to nearby energy-momentum levels.

b) The proof is similar to the proof of Theorem 2.5. We have

$$\mathrm{D}F(\bar{x}, \bar{T}, \bar{\omega}, 0, 0) = [\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x}) - \mathrm{id}, \frac{1}{\ell} f_H(\bar{x}), \xi\bar{x}, \mathrm{D}_{\lambda_E} F(\bar{y}), \mathrm{D}_{\lambda_\mu} F(\bar{y})]$$

and

$$\begin{aligned} \mathrm{D}_{\lambda_E} F(\bar{x}, \bar{T}, \bar{\omega}, \lambda_E, 0)|_{\lambda_E=0} &= \alpha \mathrm{D}_{\lambda_E} \Phi_{\bar{T}/\ell}(\bar{x}; \bar{\omega}, 0, 0), \\ \mathrm{D}_{\lambda_\mu} F(\bar{x}, \bar{T}, \bar{\omega}, 0, \lambda_\mu)|_{\lambda_\mu=0} &= \alpha \mathrm{D}_{\lambda_\mu} \Phi_{\bar{T}/\ell}(\bar{x}; \bar{\omega}, 0, 0). \end{aligned}$$

By Proposition 3.12 (see also (3.14)), $\mathrm{D}\mathbf{J}(x)$ and $\mathrm{D}H(x)$ are left eigenvectors of $\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x})$ to the eigenvalue 1 with corresponding generalized right eigenvectors t_x^μ and t_x^E and the vectors $f_H(\bar{x}) = t_x^f$ and $\xi\bar{x} = t_x^\xi$ are right eigenvectors of $\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x})$, linearly independent from t_x^μ and t_x^E. Under the non-degeneracy condition the generalized eigenspace of $\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x})$ to the eigenvalue 1 is spanned by these four vectors (see Proposition 3.12 c) (ii)). So $\mathrm{D}F(\bar{x}, \bar{T}, \bar{\omega}, 0, 0)$ has full rank if the $(2,2)$-matrix

$$B := \begin{pmatrix} \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x}; \bar{\omega}, \lambda_E, 0)|_{\lambda_E=0} & \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_\mu}\Phi_{\bar{\tau}}(\bar{x}; \bar{\omega}, 0, \lambda_\mu)|_{\lambda_\mu=0} \\ \mathrm{D}\mathbf{J}(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x}; \bar{\omega}, \lambda_E, 0)|_{\lambda_E=0} & \mathrm{D}\mathbf{J}(\bar{x})\alpha\mathrm{D}_{\lambda_\mu}\Phi_{\bar{\tau}}(\bar{x}; \bar{\omega}, 0, \lambda_\mu)|_{\lambda_\mu=0} \end{pmatrix}$$

has full rank. This can be proved similarly as (2.24): First note that $\Phi_t(\cdot;\omega) := \Phi_t(\cdot;\omega,0,0)$ conserves H and $\mathbf{J}$. This is true because $\Phi_t(\cdot;\omega) = \exp(-\omega t\xi)\Phi_t(\cdot)$, $H(\cdot)$ is Γ-invariant and $\mathbf{J}(\cdot)$ as well by (3.16), and because the flow $\Phi_t(\cdot)$ of (2.1) conserves the energy H and the momentum $\mathbf{J}$. Replacing λ by λ_E respectively λ_μ, exchanging H by $\mathbf{J}$ accordingly, replacing $\Phi_t(\cdot;\lambda)$ by $\Phi_t(\cdot;\bar{\omega},\lambda_E,0)$ or $\Phi_t(\cdot;\bar{\omega},0,\lambda_\mu)$ in (2.24) and replacing (2.20) by (3.17) in (2.21) we get

$$\begin{aligned} \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega}) &= \int_0^{\bar{\tau}} \|\mathrm{D}H(\Phi_s(\bar{x};\bar{\omega}))\|^2 \mathrm{d}s, \\ \mathrm{D}\mathbf{J}(\bar{x})\alpha\mathrm{D}_{\lambda_\mu}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega}) &= \int_0^{\bar{\tau}} \|\mathrm{D}\mathbf{J}(\Phi_s(\bar{x};\bar{\omega}))\|^2 \mathrm{d}s, \\ \mathrm{D}\mathbf{J}(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega})) &= \int_0^{\bar{\tau}} \langle \mathrm{D}H(\Phi_s(\bar{x};\bar{\omega})), \mathrm{D}\mathbf{J}(\Phi_s(\bar{x};\bar{\omega})\rangle \mathrm{d}s, \\ \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_\mu}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega}) &= \int_0^{\bar{\tau}} \langle \mathrm{D}H(\Phi_s(\bar{x};\bar{\omega})), \mathrm{D}\mathbf{J}(\Phi_s(\bar{x};\bar{\omega}))\rangle \mathrm{d}s. \end{aligned}$$

Hence for $c = (c_E, c_\mu) \in \mathbb{R}^2$ we have

$$c^T B c = \int_0^{\bar{\tau}} \|c_E \nabla H(\Phi_s(\bar{x};\bar{\omega})) + c_\mu \nabla \mathbf{J}(\Phi_s(\bar{x};\bar{\omega}))\|^2 \mathrm{d}s.$$

Since $\Phi_s(\bar{x})$, $s \in \mathbb{R}$, lies on a proper RPO $\bar{\mathcal{P}}$ (not a relative equilibrium) the vectors $\nabla H(\Phi_s(\bar{x}))$ and $\nabla \mathbf{J}(\Phi_s(\bar{x}))$ are linearly independent. Hence $c^T B c \neq 0$ for every $c \neq 0$ and

so B and the Jacobian $\mathrm{D}F(\bar{x},\bar{T},\bar{\omega},0,0)$ of (3.18) have full rank. Therefore (3.18) has a 4-dimensional solution manifold. By part a) there is a two-dimensional manifold of RPOs near $\bar{x}$ which gives a 4-dimensional manifold of solutions of (3.18) as well. So both solution manifolds coincide locally and consequently $\lambda_E = \lambda_\mu = 0$ for any solution of (3.18) close to $(\bar{\mathcal{P}},\bar{T},\bar{\omega},0,0)$.

∎

3.3.2 Continuation in energy or momentum

The RPO can be continued for example with respect to momentum and fixed energy or with respect to energy and fixed momentum. Momentum or energy are fixed by adding the constraint $F_{\bar{\mu}}(x) = \mathbf{J}(x) - \bar{\mu} = 0$ or $F_{\bar{E}}(x) = H(x) - \bar{E} = 0$ to the single shooting equation $F = 0$ from (3.18).

Proposition 3.15 *The Gauss-Newton method (2.17) applied to the equations $F^{\bar{E}} = (F, F_{\bar{E}}) = 0$ (fixed energy) and $F^{\bar{\mu}} = (F, F_{\bar{\mu}}) = 0$ (fixed momentum) converge under the conditions of Theorem 3.14.*

Proof. The proof is analogous to the proof of Proposition 2.9. By Theorem 3.14 for a non-degenerate RPO the eigenspace of $\bar{\sigma}\mathrm{D}\Phi_{\bar{T}/\ell}(\bar{x})$ to the eigenvalue 1 is 4-dimensional and $\mathrm{D}F(\bar{y})$ has a 4-dimensional kernel in the solution $\bar{y} = (\bar{x},\bar{T},\bar{\omega},0,0)$ of $F = 0$. Let

$$\begin{aligned} t^f &= (f(\bar{x}),0,0,0,0), & t^\xi &= (\xi\bar{x},0,0,0,0),\\ t^E &= (t^E_x,t^E_T,t^E_\omega,0,0), & t^\mu &= (t^\mu_x,t^\mu_T,t^\mu_\omega,0,0) \end{aligned} \tag{3.19}$$

lie in the kernel of $\mathrm{D}F(\bar{y})$ such that

$$t^E, t^\mu \in \left(\mathrm{span}(t^\xi, t^T)\right)^\perp, \quad \mathrm{D}\mathbf{J}(\bar{x})t^E_x = 0, \quad \mathrm{D}H(\bar{x})t^\mu_x = 0,$$

as in (3.14). Then

$$\mathrm{D}F_{\bar{E}}(\bar{x})t^E_x = \mathrm{D}H(\bar{x})t^E_x \neq 0, \quad \mathrm{D}F_{\bar{\mu}}(\bar{x})t^\mu_x = \mathrm{D}\mathbf{J}(\bar{x})t^\mu_x \neq 0.$$

Therefore $\mathrm{D}F^{\bar{E}}(\bar{y})$ and $\mathrm{D}F^{\bar{\mu}}(\bar{y})$ have full rank with one-dimensional kernels spanned by t^μ respectively t^E, and so the Gauss-Newton method applied to $F^{\bar{E}} = 0$ and $F^{\bar{\mu}} = 0$ converges. ∎

3.3.3 Multiple shooting ansatz

The extension of the above single shooting technique to the multiple shooting context is straightforward. We just replace $\Phi_t(\cdot;\lambda)$ in (2.28) by $\Phi_t(\cdot;\omega,\lambda_E,\lambda_\mu)$, see Sections 2.3.4 and 2.3.5. We can continue in energy and fix the momentum by adding the constraint

$$F^{\bar{\mu}}(x) = \frac{1}{k}\sum_{i=1}^{k}\mathbf{J}(x_i) - \bar{\mu} = 0$$

or we can continue in momentum and fix the energy by adding the constraint

$$F^{\bar{E}}(x) = \frac{1}{k}\sum_{i=1}^{k}H(x_i) - \bar{E} = 0.$$

Similarly to Proposition 2.14 and Proposition 3.15 we have:

Proposition 3.16 *If the RPO through $\bar{x}$ with energy $\bar{E} = H(\bar{x})$ is non-degenerate then the Gauss-Newton method (2.17) applied to $F^{\bar{E}} = (F, F_{\bar{E}}) = 0$ and $F^{\bar{\mu}} = (F, F^{\bar{\mu}}) = 0$ converge for sufficiently good enough initial data.*

3.4 Continuing periodic orbits to relative periodic orbits

In this section we show how certain RPOs bifurcating from periodic orbits in systems with symmetry group Γ of dimension greater than one can be continued numerically. By imposing spatio-temporal symmetry on the relative periodic orbits to be continued one is led back to a one-dimensional symmetry group. We use the theorem below for the continuation of relative periodic orbits of the three-body system in Section 4.

Theorem 3.17 *Let $\bar{x}$ lie on a $\bar{T}$-periodic orbit $\bar{\mathcal{P}}$ of the Hamiltonian system (2.1) with discrete spatio-temporal symmetry group L and momentum $\mathbf{J}(\bar{x}) = 0$. Let α be the drift symmetry of $\bar{\mathcal{P}}$, let K be its isotropy, let $L/K = \mathbb{Z}_\ell$ and denote by $\bar{\tau} = \bar{T}/\ell$ the relative period of the periodic orbit. Let $\tilde{L}$ be an isotropy subgroup of the action of L on 'momentum space' $\mathbf{g}^*$ such that*

$$\dim \mathrm{Fix}_{\mathbf{g}^*}(\tilde{L}) = 1 \tag{3.20}$$

and consequently also $\dim \mathrm{Fix}_{\mathbf{g}}(\tilde{L}) = 1$. Let $j \in \mathbb{N}$ be minimal such that $\alpha^j \gamma_K \in \tilde{L}$ for some $\gamma_K \in K$ and let

$$\tilde{\alpha} = \alpha^j \gamma_K, \quad \tilde{K} := K \cap \tilde{L}.$$

Since $\tilde{L}$ is finite there is some $\tilde{\ell} \in \mathbb{N}$ such that $\tilde{\alpha}^{\tilde{\ell}} \in \tilde{K}$. Let $\tilde{\ell}$ be minimal with this property and denote

$$\tilde{\tau} = j\tau, \quad \tilde{T} = \tilde{\ell}\tilde{\tau}.$$

Assume that the periodic orbit through $\bar{x}$ is non-degenerate in the sense of Definition 3.11 when considered as periodic orbit with drift symmetry $\tilde{\alpha}$, relative period $\tilde{\tau}$ and isotropy $\tilde{K}$. Then:

a) The group $\tilde{L}$ is generated by $\tilde{K}$ and $\tilde{\alpha}$, $\tilde{K}$ is normal in $\tilde{L}$ and $\tilde{L}/\tilde{K} \simeq \mathbb{Z}_{\tilde{\ell}}$.

b) There exists a 2-parameter family of RPOs, parametrized by energy E and momentum $\mu \in \mathrm{Fix}_{\mathbf{g}^*}(\tilde{L})$, $\mu \approx 0$. This family has drift velocities in $\mathrm{Fix}_{\mathbf{g}}(\tilde{L})$, relative periods close to $\tilde{\tau}$ and their spatio-temporal symmetry group at momentum 0 contains $\tilde{L}$.

c) Let ξ span $\mathrm{Fix}_{\mathbf{g}}(\tilde{L})$. Then the Gauss-Newton method (2.17) applied to (3.18) converges for initial data close to $\{(\exp(\tau\xi)\Phi_t(\bar{x}), \bar{T}, 0, 0), t \in \mathbb{R}, \tau \in \mathbb{R}\}$ if α is replaced by $\tilde{\alpha}$, ℓ by $\tilde{\ell}$, if $\Phi_t(\cdot; \omega, \lambda_E, \lambda_\mu)$ is the flow of (3.17) on $\mathrm{Fix}(\tilde{K})$ and if $\mathbf{J}$ is replaced by $\mathbf{J}_\xi$. Furthermore any solution $y = (x, T, \omega, \lambda_E, \lambda_\mu)$ of (3.18) satisfies $\lambda_E = \lambda_\mu = 0$.

Proof.

a) Let $\gamma \in \tilde{L}$. Since $\gamma \in L$ we have $\gamma = \alpha^{\tilde{j}} \tilde{\gamma}_K$ for some $\tilde{j} \in \{0, 1, \ldots, \ell - 1\}$ and $\tilde{\gamma}_K \in K$. By our assumption on j we know that $\tilde{j} \geq j$ and that $\tilde{j}$ is a multiple of j. So let $\tilde{j} = mj$. Since K is normal in L we have $\gamma = \tilde{\alpha}^m \hat{\gamma}_K$ where $\hat{\gamma}_K \in K$. From the group property of $\tilde{L}$ we conclude that $\hat{\gamma}_K \in K \cap \tilde{L} = \tilde{K}$. Hence $\tilde{L}$ is generated by $\tilde{\alpha}$ and $\tilde{K}$. For $\gamma_K \in \tilde{K}$ we have $\gamma_K \tilde{\alpha} = \tilde{\alpha}\tilde{\gamma}_K$ where $\tilde{\gamma}_K \in K$ since K is normal in L. Consequently $\tilde{\gamma}_K \in \tilde{L} \cap K = \tilde{K}$ which proves that $\tilde{K}$ is a normal subgroup of $\tilde{L}$. The definition of $\tilde{\ell}$ now implies that $\tilde{L}/\tilde{K} \simeq \mathbb{Z}_{\tilde{\ell}}$.

b) Let ξ span $\mathrm{Fix}_{\mathbf{g}}(\tilde{L})$. First note that ξ and $\tilde{\alpha}$ leave $\mathrm{Fix}(\tilde{K})$ invariant since ξ commutes with every element of $\tilde{K}$ and, by a), $\tilde{\alpha} \in N(\tilde{K})$. We consider (2.1) on $\mathrm{Fix}(\tilde{K})$ and replace Γ by the group $N(\tilde{K})/\tilde{K}$ which acts on $\mathrm{Fix}(\tilde{K})$. From now on assume without loss of generality that $\tilde{K}$ is trivial and that $\tilde{L} = \mathbb{Z}_{\tilde{\ell}}$ is generated by $\tilde{\alpha}$.

By Proposition 3.12, with $\bar{\sigma}$ replaced by $\tilde{\alpha}$, T by $\tilde{T}$ and ℓ by $\tilde{\ell}$, and because of the assumption $\dim \mathrm{Fix}_{\mathbf{g}}(\tilde{L}) = \dim \mathbf{g}_{\tilde{\alpha}} = 1$ the space of $\eta \in \mathbf{g}$ with $\eta\bar{x}$ in the kernel of

$$\tilde{\alpha} \mathrm{D}\Phi_{\tilde{T}/\tilde{\ell}}(\bar{x}) - \mathrm{id}$$

is one-dimensional and spanned by ξ. Similarly the space of row vectors $\mathrm{D}\mathbf{J}_\eta(\bar{x})$, $\eta \in \mathbf{g}$, which are left eigenvectors of $\tilde{\alpha}\mathrm{D}\Phi_{\tilde{\tau}}(\bar{x})$ to the eigenvalue 1 is one-dimensional and spanned by $\mathrm{D}\mathbf{J}_\xi(\bar{x})$. Hence the periodic orbit is non-degenerate when considered as periodic orbit with relative period $\tilde{\tau}$ and drift symmetry $\tilde{\alpha}$ when we replace Γ by the abelian group generated by $\tilde{\alpha}$ and ξ. Now part b) follows from Theorem 3.14 a).

c) Follows from part b) and Theorem 3.14 b).

■

3.5 Continuation of RPOs with regular drift-momentum pairs

In this section we consider the continuation of Hamiltonian RPOs of general compact Lie groups Γ under conditions which are generically satisfied. Namely we consider non-degenerate RPOs with regular drift-momentum pairs.

3.5.1 Persistence of Hamiltonian RPOs with regular drift-momentum pairs

We start with a definition of regular drift-momentum pairs.

Definition 3.18 *[34]*

(i) We call a drift symmetry $\sigma \in \Gamma$ regular *if* $r_\sigma = \dim \mathbf{g}_\sigma$ *is locally constant in* Γ.

(ii) We call a momentum $\mu \in \mathbf{g}^*$ regular *if* $r_\mu = \dim \mathbf{g}_\mu$ *is locally constant in* $\mathbf{g}^*$.

(iii) We call a drift-momentum pair $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$ regular *if*

$$r_{(\sigma,\mu)} = \dim \mathbf{g}_{(\sigma,\mu)}$$

is locally constant in the space of drift-momentum pairs (3.7).

Note that the space of drift-momentum pairs is in general a singular algebraic variety. As shown in [34], a drift momentum pair (σ, μ) of a compact symmetry group Γ is regular in the above sense if and only if the space of drift-momentum pairs $(\Gamma \times \mathbf{g}^*)^c$ is a manifold near (σ, μ). Moreover we have the following result which we will need later on:

Lemma 3.19 *Let* Γ *be compact. Then:*

a) If μ *is regular then* (id, μ) *is a regular drift-momentum pair.*

b) If σ *is regular then* $(\sigma, 0)$ *is a regular drift-momentum pair.*

c) The pair $(\sigma, \mu) \in (\Gamma \times \mathbf{g}^*)^c$ *is a regular drift-momentum pair if and only if* $\mathbf{g}_{(\sigma,\mu)}$ *is the Lie algebra of a Cartan subgroup and if and only if* $\mathbf{g}_{(\sigma,\mu)}$ *abelian.*

d) The set of regular momenta $\mu \in \mathbf{g}^*$ *is generic in* $\mathbf{g}^*$*, the set of regular drift symmetries is generic in* Γ *and the set of regular drift-momentum pairs are generic in the space of drift-momentum pairs* $(\Gamma \times \mathbf{g}^*)^c$.

Proof. Most of this statement is contained in [34], only the second statement of part c) is not. To prove this notice that on one hand the Lie algebra of any Cartan subgroup is abelian (see [2]). On the other hand, let $\mathbf{g}_{(\sigma,\mu)}$ be abelian. Then $\mathbf{g}_{(\sigma,\mu)}$ is the Lie algebra of a torus group in the centralizer $Z(\sigma)$ of σ. Let $\mathbb{T}$ be the maximal torus in $Z(\sigma)$ which contains this torus group. Since Γ is compact we can identify μ with an element of $\mathbf{g}$, and also with an element of $\mathbf{g}_{(\sigma,\mu)}$, see eg. [26]. Hence any element in the Lie algebra of $\mathbb{T}$ commutes with μ. Therefore the Lie algebra of $\mathbb{T}$ is contained in $\mathbf{g}_{(\sigma,\mu)}$. Thus, $\mathbf{g}_{(\sigma,\mu)}$ is the Lie algebra of a the maximal torus $\mathbb{T}$ in $Z(\sigma)$ and is therefore (see [2]) the Lie algebra of a Cartan subgroup. ∎

Example 3.20 In the case of rotational symmetry where $\Gamma = \mathrm{SO}(3)$, see Example 3.7, a drift-momentum pair $(\sigma, \mu) \in \mathrm{SO}(3) \times \mathrm{so}(3)^*$ is regular if $\mu \neq 0$ or $\sigma \neq \mathrm{id}$.

We are now ready to state a persistence result for RPOs with regular drift-momentum pair. This follows from [34, Theorem 4.2] and [34, Proposition 2.9] applied to the group $\tilde{\Gamma} := Z(\bar{\sigma})$.

Theorem 3.21 *Let $\bar{x}$ lie on a non-degenerate RPO $\bar{\mathcal{P}}$ with regular drift-momentum pair $(\bar{\sigma}, \bar{\mu}) \in (\Gamma \times \mathbf{g}^*)^c$ and let $r = r_{(\bar{\sigma},\bar{\mu})}$. Let $\bar{\tau}$ be its relative period, decompose $\bar{\sigma} = \alpha \exp(-\bar{\tau}\bar{\xi})$ as before, and let $\bar{E} = H(\bar{x}) = 0$ be the energy of the RPO. Then there is an $(r+1)$-dimensional manifold $x(E, \nu)$ of points on RPOs $\mathcal{P}(E, \nu)$ near $\bar{\mathcal{P}} = \mathcal{P}(0, 0)$ with $x(0, 0) = \bar{x}$ and*

$$\begin{array}{l} \textit{energy} \quad E, \\ \textit{momentum} \quad \bar{\mu} + \nu, \quad \nu \in \mathbf{g}^*_{(\bar{\sigma},\bar{\mu})}, \\ \textit{relative period} \quad \tau(E, \nu) \quad \textit{close to} \quad \tau(0, 0) = \bar{\tau}, \\ \textit{drift symmetry} \quad \sigma(E, \nu) \quad \textit{close to} \quad \sigma(0, 0) = \bar{\sigma}, \quad \textit{and} \\ \textit{drift velocity} \quad \xi(E, \nu) \in \mathbf{g}_{(\bar{\sigma},\bar{\mu})} \quad \textit{close to} \quad \xi(0, 0) = \bar{\xi} \end{array}$$

such that $\sigma(E, \nu) = \alpha \exp(-\tau(E, \nu)\xi(E, \nu))$. Moreover all RPOs close to $\bar{x}$ with relative period close to $\bar{\tau}$ and drift symmetry close to $\bar{\sigma}$ belong to this family of RPOs.

The space $\bar{\mu} + (\mathbf{g}\bar{\mu})^\perp$ is a section transverse to the momentum group orbit $\Gamma\bar{\mu}$ at $\bar{\mu}$ in momentum space $\mathbf{g}^*$. Since $(\mathbf{g}\bar{\mu})^\perp \simeq \mathbf{g}^*_{\bar{\mu}}$ we can therefore interpret $\mathbf{g}^*_{\bar{\mu}}$ as transverse section to $\Gamma\bar{\mu}$ as well. Moreover the elements of $\mathbf{g}^*_{(\bar{\sigma},\bar{\mu})} = \mathrm{Fix}_{\mathbf{g}^*_{\bar{\mu}}}(\bar{\sigma})$ are the momenta in the transverse section $\mathbf{g}^*_{\bar{\mu}}$ which are fixed by the drift symmetry $\bar{\sigma}$. Theorem 3.21 therefore says that near a non-degenerate RPO with regular drift-momentum pair there is a family of RPOs parametrized by energy and those momenta which are fixed by the drift symmetry of the original RPO in a section transverse to the momentum group orbit of the original RPO.

Due to our assumption of non-degeneracy of the RPO $\bar{\mathcal{P}}$ we can parametrize all RPOs near the given RPO $\bar{\mathcal{P}}$ with relative period close to $\bar{\tau}$ by their energy and by their drift-momentum pairs which in general form a singular algebraic variety. The assumption of a regular drift-momentum pair ensures that this variety is locally a manifold and enables us to use an implicit function type argument to prove the existence of a manifold of RPOs near the given RPO $\bar{\mathcal{P}}$, see [34] for more details.

3.5.2 Equivalent parametrization by drift velocity and relative period

The parametrization of the manifold of RPOs of Theorem 3.21 by energy E and momentum $\bar{\mu} + \nu$, $\nu \in \mathbf{g}^*_{(\bar{\sigma},\bar{\mu})}$, is equivalent to the parametrization by velocity $\xi \in \mathbf{g}_{(\bar{\sigma},\bar{\mu})}$ and relative period τ under the assumption that the determinant of the matrix

$$\begin{pmatrix} \partial_E \xi(E, \nu) & \partial_\nu \xi(E, \nu) \\ \partial_E \tau(E, \nu) & \partial_\nu \tau(E, \nu) \end{pmatrix} \tag{3.21}$$

does not vanish. This assumption is satisfied at $(E,\nu)=(0,0)$, that is, at the RPO through $\bar{x}$ if the corresponding block in the linearization $\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ of the RPO has full rank: Let X_1 be the generalized eigenspace of $M=\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})$ to the eigenvalue 1 and let P_1 be the corresponding spectral projection of X_1 and $M_1=P_1M|_{X_1}$. Choose coordinates on X_1 such that $\mathbf{g}_{(\bar{\sigma},\bar{\mu})}\bar{x}$ is spanned by the first $r=r_{(\bar{\sigma},\bar{\mu})}$ unit vectors $e_1,\ldots,e_r$, such that $\mathbf{g}_{\bar{\sigma}}\bar{x}$ is spanned by the first $s=r_{\bar{\sigma}}$ unit vectors $e_1,\ldots,e_s$ and such that $f_H(\bar{x})$ is parallel to e_{s+1}. Moreover assume that $e_{s+2}^T,\ldots,e_{r+s+1}^T$ span the space of row vectors $\mathrm{D}\mathbf{J}_\xi(\bar{x})$, $\xi\in\mathbf{g}_{(\bar{\sigma},\bar{\mu})}$, and that $\mathrm{D}H(\bar{x})$ is parallel to e_{r+s+2}^T. By Proposition 3.12 the matrix M_1 takes the form

$$M_1=\begin{pmatrix}\mathrm{id}_s & 0 & * & *\\ 0 & 1 & * & *\\ 0 & 0 & \mathrm{id}_r & 0\\ 0 & 0 & 0 & 1\end{pmatrix} \tag{3.22}$$

where id_n is the n-dimensional identity matrix. Denote the submatrix of (3.22) formed of the stars by $\tilde{B}$ and let B be the $(r+1,r+1)$-matrix $B=\tilde{P}\tilde{B}$ where $\tilde{P}$ is the projection onto the space spanned by $e_1,\ldots,e_r,e_{s+1}$. Then we obtain

Lemma 3.22 *The matrix* (3.21) *has full rank at* $(E,\nu)=(0,0)$ *if the matrix* B *has full rank.*

Proof. Differentiating the fixed point equation $\sigma(E,\nu)\Phi_{\tau(E,\nu)}(x(E,\nu))=x(E,\nu)$ at $(E,\nu)=(0,0)$ and applying P_1 we get

$$\begin{aligned}0 &= (M_1-\mathrm{id})P_1\mathrm{D}_{(E,\nu)}x(E,\nu)|_{(E,\nu)=(0,0)}+\mathrm{D}_{(E,\nu)}\tau(E,\nu)|_{(E,\nu)=(0,0)}(f_H(\bar{x})-\bar{\xi}\bar{x})\\ &\quad -\bar{\tau}\mathrm{D}_{(E,\nu)}\xi(E,\nu)|_{(E,\nu)=(0,0)}\bar{x}.\end{aligned}$$

Let P be the projection onto X_1 and then onto the span of the vectors e_j, $j=s+1,\ldots,r+s+2$, of X_1. Then

$$\begin{aligned}0 &= BP\,\mathrm{D}_{(E,\nu)}x(E,\nu)|_{(E,\nu)=(0,0)}+\mathrm{D}_{(E,\nu)}\tau(E,\nu)|_{(E,\nu)=(0,0)}(f_H(\bar{x})-\bar{\xi}\bar{x})\\ &\quad -\bar{\tau}\mathrm{D}_{(E,\nu)}\xi(E,\nu)|_{(E,\nu)=(0,0)}\bar{x}.\end{aligned}$$

The parametrization of the manifold of RPOs by (E,ν) from Theorem 3.21 implies that the $(r+1,r+1)$-matrix $P\,\mathrm{D}_{(E,\nu)}x(E,\nu)|_{(E,\nu)=(0,0)}$ has full rank. Therefore the $(r+1,r+1)$-matrix

$$\begin{pmatrix}-\bar{\tau}\partial_E\xi(E,\nu)-\partial_E\tau(E,\nu)\bar{\xi} & -\bar{\tau}\partial_\nu\xi(\nu,E)-\partial_\nu\tau(E,\nu)\bar{\xi}\\ \partial_E\tau(E,\nu) & \partial_\nu\tau(E,\nu)\end{pmatrix}\Big|_{(E,\nu)=(0,0)}$$

has full rank. By elementary row operations this matrix can be transformed into the matrix (3.21) which therefore also has full rank. ∎

3.5.3 Numerical computation of RPOs with regular drift-momentum pair

Let $\bar{x}$ lie on a non-degenerate RPO $\bar{\mathcal{P}}$ with relative period $\bar{\tau}$ and regular drift-momentum pair $(\bar{\sigma},\bar{\mu})\in\Gamma\times\mathbf{g}^*$ where $\bar{\sigma}=\alpha\exp(-\bar{\tau}\bar{\xi})$. Let $\Gamma_\sigma=Z(\sigma)$ as in (3.8) and define $\Gamma_{(\sigma,\mu)}=Z(\sigma)\cap\Gamma_\mu$ as in (3.10). Denote, as before, $r=r_{(\bar{\sigma},\bar{\mu})}$, let $\xi_1,\ldots,\xi_r$ be a basis of $\mathbf{g}_{(\bar{\sigma},\bar{\mu})}$, let $s=r_{\bar{\sigma}}$, let $\xi_1,\ldots,\xi_s$ be a basis of $\mathbf{g}_{\bar{\sigma}}$ and let $\bar{\xi}=\sum_{i=1}^r\bar{\omega}_i\xi_i$. Note that by Lemma 3.19 d) generically $\bar{\sigma}$ is regular and $s=r$.

Define

$$\dot{x}=f_H(x)+\lambda_E\nabla H(x)+\sum_{i=1}^r\lambda_{\mu,i}\nabla\mathbf{J}_{\xi_i}(x)-\sum_{i=1}^s\omega_i\xi_i. \tag{3.23}$$

Then the following theorem holds true:

Theorem 3.23 *Let $\bar{x}$ lie on a non-degenerate RPO $\bar{\mathcal{P}}$ with relative period $\bar{\tau}$, and with regular drift-momentum pair $(\bar{\sigma},\bar{\mu})\in\Gamma\times\mathbf{g}^*$ where $\bar{\sigma}=\alpha\exp(-\bar{\tau}\bar{\xi})$ is decomposed as in Lemma 3.9 and let $r=r_{(\bar{\sigma},\bar{\mu})}$, $\bar{T}=\ell\bar{\tau}$. Denote by $\Phi_t(x;\omega,\lambda_E,\lambda_\mu)$ the flow of (3.23). Then the following holds true:*

a) the Gauss-Newton method (2.17) applied to

$$F(x,T,\omega,\lambda_E,\lambda_\mu)=\alpha\Phi_{\frac{T}{\ell}}(x;\omega,\lambda_E,\lambda_\mu)-x,\quad F:X\times\mathbb{R}^{2+s+r}\subseteq\mathbb{R}^{n+2+s+r}\to\mathbb{R}^n \tag{3.24}$$

converges for initial values $y=(x,T,\omega,\lambda_E,\lambda_\mu)$ close to

$$\{(\gamma\Phi_t(\bar{x}),\bar{T},\bar{\omega},0,0),\quad t\in\mathbb{R},\ \gamma\in\Gamma_{(\bar{\sigma},\bar{\mu})}\}. \tag{3.25}$$

b) Any solution $y=(x,T,\omega,\lambda_E,\lambda_\mu)$ of $F=0$ close to the set (3.25) satisfies $\lambda_E=0$, $\lambda_\mu=0$. Hence it is an RPO of (2.1).

Proof. We replace Γ by $\Gamma_{\bar{\sigma}}=Z(\bar{\sigma})$ and consequently look for RPOs with drift velocity $\xi=\sum_{i=1}^s\omega_i\xi_i\in\mathbf{g}_{\bar{\sigma}}$.

a) The matrix

$$\begin{aligned}\mathrm{D}F(\bar{x},\bar{T},\bar{\omega},0,0) &= [\mathrm{D}_xF,\mathrm{D}_TF,\mathrm{D}_\omega F,\mathrm{D}_{\lambda_E}F,\mathrm{D}_{\lambda_\mu}F]\\ &= [\bar{\sigma}\mathrm{D}\Phi_{\bar{\tau}}(\bar{x})-\mathrm{id},f_H(\bar{x}),\xi_1\bar{x},\dots,\xi_s\bar{x},\mathrm{D}_{\lambda_E}F,\mathrm{D}_{\lambda_\mu}F]\end{aligned}$$

has full rank if the $(r+1,r+1)$-matrix B with

$$\begin{aligned}B_{ij} &= \mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})\mathrm{D}_{\lambda_{\mu,j}}F(\bar{y}) = \mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})\alpha\mathrm{D}_{\lambda_{\mu,j}}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega},0,\lambda_\mu)|_{\lambda_\mu=0},\\ &\qquad i,j=1,\dots,r,\\ B_{i,r+1} &= \mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})\mathrm{D}_{\lambda_E}F(\bar{y}) = \mathrm{D}\mathbf{J}_{\xi_i}(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega},\lambda_E,0)|_{\lambda_E=0},\\ &\qquad i=1,\dots,r,\\ B_{r+1,i} &= \mathrm{D}H(\bar{x})\mathrm{D}_{\lambda_{\mu,i}}F(\bar{y}) = \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_{\mu,i}}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega},0,\lambda_\mu)|_{\lambda_\mu=0},\\ &\qquad i=1,\dots,r,\\ B_{r+1,r+1} &= \mathrm{D}H(\bar{x})\mathrm{D}_{\lambda_E}F(\bar{y}) = \mathrm{D}H(\bar{x})\alpha\mathrm{D}_{\lambda_E}\Phi_{\bar{\tau}}(\bar{x};\bar{\omega},\lambda_E,0)|_{\lambda_E=0}\end{aligned}$$

has full rank. Since $(\bar{\sigma},\bar{\mu})$ is regular the isotropy algebra $\mathbf{g}_{(\bar{\sigma},\bar{\mu})}$ is abelian by Lemma 3.19 c). Consequently, $\Phi_t(\cdot;\omega)=\exp(-t\sum_{i=1}^r\omega_i\xi_i)\Phi_t(\cdot)$ conserves the momenta $\mathbf{J}_{\xi_j}$, $j=1,\dots,r$. Therefore we can show that B has full rank in the same way as in the proof of Theorem 3.14. Hence $\mathrm{D}F(\bar{x},\bar{T},\bar{\omega},0,0)$ has full rank and $F=0$ has a $(2+r+s)$-dimensional family of solutions.

Since $\Gamma_{(\bar{\sigma},\bar{\mu})}\subseteq Z(\bar{\sigma})$ and $Z(\bar{\sigma})=Z(\alpha)\cap Z(\bar{\xi})$ by Lemma 3.9, the points $\gamma\Phi_t(\bar{x})$, $t\in\mathbb{R}$, $\gamma\in Z(\bar{\sigma})$, lie on an RPO with drift velocity $\bar{\xi}$, and so the set (3.25) consists of solutions of $F=0$. By $\Gamma_{(\bar{\sigma},\bar{\mu})}$-equivariance and time-shift equivariance the above convergence argument also holds true at all points in the set (3.25), and so the Gauss-Newton method converges for initial data close to (3.25).

b) We proved in part a) that the equation $F=0$ has an $(s+r+2)$-dimensional solution manifold near the set (3.25). By Theorem 3.21 there is an $(r+1)$-dimensional manifold $x(E,\nu)$ of points on RPOs $\mathcal{P}(E,\nu)$ of (2.1) near $\bar{x}$ with drift symmetries $\sigma(E,\nu)\in\Gamma_{(\bar{\sigma},\bar{\mu})}$ and period $T(E,\nu)=\ell\tau(E,\nu)$ in a frame moving with velocity $\xi(E,\nu)$. Let $\xi(E,\nu)=\sum_{i=1}^r\omega_i(E,\nu)\xi_i$. As in part a) we see that with $x(E,\nu)$ also $(\gamma\Phi_t(x(E,\nu)),T(E,\nu),\omega(E,\nu),0,0)$, $t\in\mathbb{R}$, $\gamma\in Z(\bar{\sigma})$, is a solution of $F=0$. This gives an $(r+s+2)$-dimensional manifold of solutions of $F=0$ which are RPOs of (2.1). Hence the $(r+s+2)$-dimensional solution manifold of $F=0$ near (3.25) consists of RPOs of (2.1) and satisfies $\lambda_E=\lambda_\mu=0$.

Remarks 3.24

a) Theorems 3.21 and 3.23 can also be applied to compute certain bifurcating RPOs with smaller isotropy and larger relative period (and hence smaller spatio-temporal symmetry in a comoving frame): Let K be the isotropy of the point $\bar{x}$ of the RPO $\bar{\mathcal{P}}$, let $\bar{\sigma}$ be its drift symmetry, $\bar{\tau}$ be its relative period, let $\tilde{K}$ be a subgroup of K and let $N(\tilde{K})$ be the normalizer of $\tilde{K}$. To search for RPOs near $\bar{\mathcal{P}}$ with isotropy subgroup $\tilde{K}$ we restrict the dynamics to $\mathrm{Fix}(\tilde{K})$ instead of $\mathrm{Fix}(K)$, c.f. Remark 2.2. Decompose $\bar{\sigma} = \alpha \exp(-\bar{\tau}\bar{\xi})$ as in Lemma 3.9. Then $\bar{\sigma}^\ell = \exp(-\bar{T}\bar{\xi}) \in Z(K)$, see Remark 3.10. Hence there are $j \in \{1, 2, \ldots, \ell\}$, $\gamma_K \in K$, such that $\sigma^j \gamma_K \in N(\tilde{K})$. Let $j > 0$ be minimal with this property. We now replace Γ by the symmetry group $\tilde{\Gamma} = N(\tilde{K})/\tilde{K}$ acting on $\mathrm{Fix}(\tilde{K})$. Then we can consider the RPO $\bar{\mathcal{P}}$ as RPO with drift symmetry $\tilde{\sigma} = \bar{\sigma}^j \gamma_K$ and relative period $\tilde{\tau} = j\bar{\tau}$ on $\mathrm{Fix}(\tilde{K})$ and can apply Theorems 3.21 and 3.23 to continue it in energy and momentum provided that the non-degeneracy condition is satisfied and $\tilde{\sigma}$ is a regular drift-momentum pair for $\tilde{\Gamma}$. The bifurcating RPOs have isotropy containing $\tilde{K}$ and relative period close to $\tilde{\tau}$.

b) Theorem 3.17 is a corollary of Theorems 3.21 and 3.23 and part a) of this remark: In this case the RPO is a periodic orbit, i.e., $\bar{\xi} = 0$, $\bar{\sigma} = \alpha$, with momentum $\bar{\mu} = 0$. We now treat the periodic orbit as an RPO of relative period $\tilde{\tau} = j\bar{\tau}$ and drift symmetry $\tilde{\sigma} = \tilde{\alpha} = \bar{\sigma}^j \gamma_K$ on $\mathrm{Fix}(\tilde{K})$ as in a). By Lemma 3.19 c) the pair $(\tilde{\alpha}, 0)$ is a regular drift-momentum pair if and only if $\mathbf{g}_{(\tilde{\alpha},0)} = \mathbf{g}_{\tilde{\alpha}}$ is abelian. Condition (3.20) implies that $\mathbf{g}_{\tilde{\alpha}}$ is one-dimensional and hence abelian, so $(\tilde{\alpha}, 0)$ is a regular drift-momentum pair and $r = 1$ in Theorems 3.21 and 3.23.

3.5.4 Continuation of branches of RPOs

By Theorem 3.21 there is an $(r+1)$-dimensional manifold of RPOs near a non-degenerate RPO with regular drift-momentum pair $(\bar{\sigma}, \bar{\mu})$, where $r = r_{(\bar{\sigma},\bar{\mu})}$. Let, as before, $\xi_1, \ldots, \xi_r$ be a basis of $\mathbf{g}_{(\bar{\sigma},\bar{\mu})}$ and denote $\mathbf{J}_i = \mathbf{J}_{\xi_i}$. To select a branch of RPOs one can for example fix $r-1$ of the first r components of the momentum map (without loss of generality the first $r-1$ components) and the energy

$$F_{\bar{\mu}_i}(x) = \mathbf{J}_i(x) - \bar{\mu}_i = 0, \quad i = 1, \ldots, r-1, \quad F_{\bar{E}}(x) = H(x) - \bar{E} = 0,$$

and then the RPOs are continued with respect to the conserved quantity $\mathbf{J}_r$. Another option is to fix the first r components of the momentum map and continue the RPOs with respect to energy. These constraints have to be added to F from (3.24).

The following proposition is analogous to Proposition 3.15.

Proposition 3.25 *Let the assumptions of Theorem 3.21 hold. Then the Gauss-Newton method (2.17) applied to the equations $F^{\bar{E}} = (F, F_{\bar{E}}, F_{\bar{\mu}_1}, \ldots, F_{\bar{\mu}_{r-1}}) = 0$ (continuation of RPOs in the momentum component $\mathbf{J}_r$ with fixed energy and fixed momentum components $\mathbf{J}_1, \ldots, \mathbf{J}_{r-1}$) converges. The same holds true for the Gauss-Newton method applied to the equations $F^{\bar{\mu}} = (F, F_{\bar{\mu}}) = 0$, where $F_{\bar{\mu}} = (F_{\bar{\mu}_1}, \ldots, F_{\bar{\mu}_r})$ (continuation of RPOs in energy with fixed momentum).*

Proof. Since the RPO is non-degenerate the Jacobian $\mathrm{D}F(\bar{y})$ of (3.24) has a $(2+s+r)$-dimensional kernel spanned by the vectors, $t^{\xi_1}, \ldots, t^{\xi_s}, t^f, t^{\mu_1}, \ldots, t^{\mu_r}, t^E$ where

$$t^{\xi_i} = (\xi_i \bar{x}, 0, 0, 0, 0), \quad i = 1, \ldots, r, \quad t^f = (f_H(\bar{x}), 0, 0, 0, 0)$$

as in (3.19). The x-components of the vectors $t^{\mu_i} = (t_x^{\mu_i}, t_T^{\mu_i}, t_\omega^{\mu_i}, 0, 0)$ and $t^E = (t_x^E, t_T^E, t_\omega^E, 0, 0)$ can be chosen to satisfy (3.14). From (3.14) we conclude that

$$\begin{aligned} &\mathrm{D}F_{\bar{E}}(\bar{x})t^E = 1, \qquad &&\mathrm{D}F_{\bar{\mu}_i}(\bar{x})t_x^{\mu_j} = \delta_{ij}, \quad i,j = 1,\dots,r, \\ &\mathrm{D}F_{\bar{\mu}_i}(\bar{x})t_x^E = 0, \qquad &&\mathrm{D}F_{\bar{E}}(\bar{x})t_x^{\mu_i} = 0, \quad i = 1,\dots,r. \end{aligned} \tag{3.26}$$

Therefore $\mathrm{D}F^{\bar{E}}(\bar{y})$ and $\mathrm{D}F^{\bar{\mu}}(\bar{y})$ have full rank with kernel spanned by t^{μ_r} and t^E respectively and the Gauss-Newton method applied to $F^{\bar{E}} = 0$ and $F^{\bar{\mu}} = 0$ converges. ∎

The extension to the multiple shooting context is straightforward.

Remark 3.26 In [15, 29] Galán et al numerically continue periodic orbits of symmetric Hamiltonian systems without exploiting spatio-temporal symmetries, i.e., they set $\alpha = \mathrm{id}$, $\bar{\xi} = 0$, $\ell = 1$. Their numerical methods converge if the geometric multiplicity of the eigenvalue 1 of $\mathrm{D}\Phi_{\bar{T}}(\bar{x})$ (where $\bar{x}$ lies on a $\bar{T}$-periodic orbit) is $\dim\Gamma + 1$ (see [29, Theorem 14]). Under this condition there is a locally unique periodic orbit through $\bar{x}$ with fixed period $\bar{T}$ which can be continued with respect to an external parameter. Numerically they compute this periodic orbit by a Newton method as the solution of the equation

$$0 = F(x, \lambda_E, \lambda_\mu), \quad F : X \times \mathbb{R}^{1+g} \subseteq \mathbb{R}^{n+1+g} \to \mathbb{R}^{n+1+g}$$

where $g = \dim\Gamma$, $\xi_1, \dots, \xi_g$ is a basis of $\mathbf{g}$, and

$$F(x, \lambda_E, \lambda_\mu) = \begin{pmatrix} \Phi_{\bar{T}}(x; \lambda_E, \lambda_\mu) - x \\ \langle x - \bar{x}, f_H(\bar{x})\rangle \\ \langle x - \bar{x}, \xi_1 \bar{x}\rangle \\ \vdots \\ \langle x - \bar{x}, \xi_g \bar{x}\rangle \end{pmatrix}.$$

In contrast, we allow for periodic orbits to be continued as RPOs. For our pathfollowing method to converge we require that the RPOs to be continued are non-degenerate, a condition which is different from, but related to the condition that Muñoz-Almaraz et al require, see Proposition 3.12. Our method provides continuation in momentum and energy as well continuation in an external parameter (c.f. Remark 2.10 a). Since we want to continue in momentum, we need the additional condition that the drift-momentum pair of the RPO is regular; if this condition fails then the set of RPOs near a given RPO is not a manifold any more, c.f. [34].

4 Continuation of rotating choreographies

In this section we show how Theorem 3.17 can be applied to periodic orbits of N-body problems, and in particular to choreographies.

4.1 N-body problems

We consider N identical bodies of mass 1 in $\mathbb{R}^3$ acted on only by the forces they exert on each other. These forces are assumed to be given by $\frac{1}{2}N(N-1)$ identical copies of a potential energy function V (one for each pair of bodies) which depends only on the distance between the bodies. Writing p_j for the momenta conjuate to the positions q_j, $q = (q_1, \dots, q_N)$, $p = (p_1, \dots, p_N)$, the Hamiltonian is

$$H(q,p) = \frac{1}{2}\sum_{j=1}^{N} |p_j|^2 + \sum_{i<j} V(r_{ij}) \quad \text{where} \quad r_{ij} = |q_i - q_j|, \quad V(r) = -\frac{1}{r}. \tag{4.1}$$

Excluding collisions, the configuration space Q is

$$Q = \{q = (q_1, \ldots, q_N) \in \mathbb{R}^{3(N-1)}, \quad q_i \neq q_j \ \text{ for } i \neq j\}$$

and the phase space is $P = Q \times \mathbb{R}^{3N} \subset \mathbb{R}^{6N}$. The equations of motion are

$$\dot{q}_j \ = \ p_j, \qquad \dot{p}_j \ = \ \sum_{i \neq j} \frac{q_i - q_j}{r_{ij}^3}, \qquad j = 1, \ldots, N. \tag{4.2}$$

The angular momentum is $\mathbf{J}(q,p) = \sum_{j=1}^{N} q_j \wedge p_j$. Without loss of generality, the centre of mass of the systems can be assumed to be fixed at 0 restricting the configuration space to

$$Q^0 \ = \ \{q \in Q \ : \ \sum_{j=1}^{N} q_j = 0\}$$

with corresponding phase space $P^0 = Q^0 \times \mathbb{R}^{3(N-1)} \subseteq \mathbb{R}^{6(N-1)}$.

4.2 Example: three-body system with fixed centre of mass

As a specific example we consider the three-body problem. The phase space is then $P^0 \subseteq \mathbb{R}^{12}$ with $x \in P^0$ given by $x = (q_1, q_2, p_1, p_2) \in P^0$, $q_i \in \mathbb{R}^3$, $p_i \in \mathbb{R}^3$, $i = 1, 2$. The third particle satisfies $q_3 = -q_1 - q_2$, $p_3 = -p_1 - p_2$ because the centre of mass is fixed at 0 and so the global linear momentum vanishes (i.e., $p_1 + p_2 + p_3 = 0$). Then the Hamiltonian is given by

$$H^0 = \frac{1}{2}\left(|p_1|^2 + |p_2|^2 + |p_1 + p_2|^2\right) + V^0(q) \tag{4.3}$$

where the potential $V^0(q)$ is

$$\begin{aligned} V^0(q) \ &= \ -\frac{1}{|q_1 - q_2|} - \frac{1}{|q_1 - (-q_1 - q_2)|} - \frac{1}{|q_2 - (-q_1 - q_2)|} \\ &= \ -\frac{1}{|q_1 - q_2|} - \frac{1}{|2q_1 + q_2|} - \frac{1}{|2q_2 + q_1|}. \end{aligned}$$

Inserting $q_3 = -q_1 - q_2$ and $p_3 = -p_1 - p_2$ into the symplectic form (2.2) the standard symplectic structure matrix from (2.3) transforms into the symplectic structure matrix $\mathbb{J}^0$ with

$$\mathbb{J}^0 = \begin{pmatrix} 0 & \mathbb{J}_6 \\ -\mathbb{J}_6 & 0 \end{pmatrix}, \quad \text{where } \ \mathbb{J}_6 = \frac{1}{3}\begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix} \otimes \mathrm{id}_3.$$

The equations of motion are given by (4.2) with $N = 3$ and q_3, p_3 replaced by $-q_1 - q_2$ and $-p_1 - p_2$ respectively:

$$\begin{aligned} \dot{q}_1 \ &= \ p_1, \ \ \dot{p}_1 = -\left(\frac{q_1 - q_2}{|q_1 - q_2|^3} + \frac{2q_1 + q_2}{|2q_1 + q_2|^3}\right), \\ \dot{q}_2 \ &= \ p_2, \ \ \dot{p}_2 = -\left(\frac{q_2 - q_1}{|q_1 - q_2|^3} + \frac{2q_2 + q_1}{|2q_2 + q_1|^3}\right). \end{aligned}$$

4.3 Symmetries of N-body problems

The N-identical-body Hamiltonian (4.1) has the following symmetries:

1. *Rotations and reflections of* $\mathbb{R}^3$*:* These form the orthogonal group O(3) which acts diagonally on the positions and velocities:

$$R(q_1,\ldots,q_N,p_1,\ldots,p_N) \;=\; (Rq_1,\ldots,Rq_N,Rp_1,\ldots,Rp_N) \quad R\in \mathrm{O}(3),\; q_j,p_j\in\mathbb{R}^3.$$

   We define the *symmetry axis* of a rotational symmetry to be its usual rotation axis and that of a reflectional symmetry to be the axis perpendicular to the reflection plane. In the following let $\kappa_i \in \mathrm{O}(3)$ be the reflection with symmetry axis e_i, i.e., let κ_i be such that $\kappa_i e_i = -e_i$, $\kappa_i e_j = e_j$ for $j \neq i$, $i,j = 1,2,3$.

2. *Permutations of identical bodies:* Because we assume that all the bodies are identical the Hamiltonian is also invariant under the action of S_N, the group of all permutations of the integers $1,\ldots,N$:

$$\pi.(q_1,\ldots,q_N,\dot q_1,\ldots,\dot q_N) \;=\; (q_{\pi(1)},\ldots,q_{\pi(N)},p_{\pi(1)},\ldots,p_{\pi(N)}) \quad \pi\in S_N,\; q_j,p_j\in\mathbb{R}^3.$$

   In the following we will frequently use the notation $\pi = (\pi(1),\ldots,\pi(N))$.

Taken together these three symmetry groups give an action of

$$\Gamma = \mathrm{O}(3)\times S_N$$

on P which reduces to an action on P^0 and leaves the Hamiltonian (4.1) invariant.

Remark 4.1 We call a matrix $\rho \in \mathrm{GL}(n)$ of a general Hamiltonian system (2.1) a *time-reversing symmetry* of (2.1) if

$$H(\rho x) = H(x), \quad x\in X, \quad \rho\mathbb{J} = -\mathbb{J}\rho.$$

This implies that $f_H(\rho x) = -\rho f_H(x)$, $x\in X$, and so with $x(t)$ also $\rho x(-t)$ is a solution of (2.1). In addition to the symmetries listed above, the N-body system (4.2) has the *time-reversing symmetry*

$$\rho.(q_1,\ldots,q_N,p_1,\ldots,p_N) \;=\; (q_1,\ldots,q_N,-p_1,\ldots,-p_N) \qquad q_j,p_j\in\mathbb{R}^3$$

which generates a group $\mathbb{Z}_2(\rho)$ of order 2.

Since S_N is finite the Lie algebra of Γ is just $\mathbf{g} = \mathrm{so}(3)$, the Lie algebra of SO(3), which we can identify with $\mathbb{R}^3$, see (3.4). The adjoint action of O(3) on so(3) is

$$\mathrm{Ad}_R\xi \;=\; \det(R)R\xi$$

where on the right $R\in\mathrm{O}(3)$ is identified with a 3×3 orthogonal matrix and ξ with a vector in $\mathbb{R}^3$. Since S_N commutes with O(3) it acts trivially in the adjoint action of Γ on $\mathbf{g}$. As Γ is compact its adjoint and coadjoint actions coincide and so the coadjoint action of Γ on $\mathbf{g}^* \simeq \mathrm{so}(3)^*$ is

$$\gamma\mu = (R,\pi)\mu = \det(R)R\mu, \quad \gamma = (R,\pi)\in\Gamma = \mathrm{O}(3)\times S_N.$$

Note in particular that rotations and reflections in O(3) both act like rotations on the angular velocity vectors $\xi\in\mathrm{so}(3)$, the reflections giving rotations by 180 degree about axes perpendicular to their reflection planes in physical space.

Definition 4.2 *A periodic orbit of (4.2) is a* choreography *if all the bodies follow the same path in* $\mathbb{R}^3$*, separated only by a phase shift. This is equivalent to requiring that the spatio-temporal symmetry group* L *of the periodic orbit contains an order* N *cyclic permutation* $\pi\in S_N$ *which can always be taken to act on* Q *by* $\pi q = (q_2,q_3,\ldots,q_N,q_1)$*. Similarly a relative periodic orbit of (4.2) with angular velocity* ξ *is a rotating choreography if it is a choreography in coordinates rotating with velocity* ξ*.*

We say that $R\in\mathrm{SO}(3)$ and $\hat R\in\mathrm{O}(3)\setminus\mathrm{SO}(3)$ are rotational and reflectional symmetries of a periodic orbit if they are spatio-temporal symmetries of this periodic orbit.

4.4 Persistence of rotating choreographies

We are now ready to state the following persistence result for rotating choreographies. This result generalizes a theorem on rotating Eights by Chenciner et al [4] from three bodies to the case of N bodies and combines the persistence result with the convergence of the numerical scheme. Montaldi and Roberts [28] obtained an analogous persistence result for relative equilibria of molecules bifurcating from equilibria.

Corollary 4.3 *Let $\bar{x}$ lie on a periodic orbit $\bar{\mathcal{P}}$ of the N-body problem (4.2) in $\mathbb{R}^3$ with period $\bar{T}$, energy $\bar{E} = H(\bar{x}) = 0$, and angular momentum $\mathbf{J}(\bar{x}) = 0$. Then:*

a) Under some non-degeneracy assumption (see d)) for each reflectional or rotational symmetry of the periodic orbit there is a 2-parameter bifurcating family $\mathcal{P}(E,\nu)$ of relative periodic orbits smoothly parametrized by energy $H(x(E,\nu)) = E$ and angular momentum $\nu = \mathbf{J}_\xi(x(E,\nu))$ such that $x(E,\nu) \in \mathcal{P}(E,\nu)$ and $x(0,0) = \bar{x}$. The family of RPOs has angular velocity and angular momentum parallel to the symmetry axis $\xi \in \mathrm{so}(3) \simeq \mathrm{so}(3)^* \simeq \mathbb{R}^3$.

b) The reflectional and rotational symmetries of the periodic orbit $\bar{\mathcal{P}}$ which also fix the symmetry axis ξ persist as symmetries of the corresponding family of RPOs from a). More precisely we have:

(i) The isotropy subgroup $\tilde{K}$ of the family of RPOs from a) is

$$\tilde{K} = \{\gamma \in K, \quad \mathrm{Ad}_\gamma \xi = \xi\}$$

where K is the isotropy subgroup of the periodic orbit $\bar{\mathcal{P}}$.

(ii) Let α be the drift symmetry of the periodic orbit through $\bar{\mathcal{P}}$, let $\bar{\tau}$ be its relative period, let K be its isotropy and choose $j \in \mathbb{N}$ minimal such that $\tilde{\alpha} := \alpha^j \gamma_K$ satisfies $\mathrm{Ad}_{\tilde{\alpha}} \xi = \xi$ for some $\gamma_K \in K$. Then the family of RPOs from a) has drift symmetry close to $\tilde{\alpha}$ and relative period close to $\tilde{\tau} = j\bar{\tau}$.

Moreover all RPOs near $\bar{\mathcal{P}}$ with such drift symmetry, angular velocity and relative period belong to this family.

c) If the periodic orbit $\bar{\mathcal{P}}$ is a choreography then the bifurcating RPOs are rotating choreographies.

d) The non-degeneracy condition we require is that the periodic orbit $\bar{\mathcal{P}}$ is non-degenerate when considered as periodic orbit on $\mathrm{Fix}(\tilde{K})$ with the symmetry data from b). Under these conditions, with these symmetry data and with $\tilde{\ell}$ and $\tilde{T}$ as in Theorem 3.17 the Gauss-Newton method (2.17) applied to (3.18) converges.

Proof. Let L be the spatio-temporal symmetry group of the periodic orbit $\bar{\mathcal{P}}$, let $R \in L$ be a reflectional or rotational symmetry of $\bar{\mathcal{P}}$ with symmetry axis $\xi \in \mathrm{so}(3)$ and let $\tilde{L} = \{\gamma \in \Gamma, \mathrm{Ad}_\gamma \xi = \xi\}$. Since reflectional and rotational symmetries have a one dimensional fixed point space in $\mathrm{so}(3)^*$ there is, by Theorem 3.17, a two-parameter family $x(E,\nu)$ of RPOs with angular momentum fixed by R. This gives part a) and b). For part c) let L contain the cyclic permutation π, i.e., let $\bar{\mathcal{P}}$ be a choreography. Since the symmetries in S_N act trivially on $\mathrm{so}(3)^*$ also every isotropy subgroup $\tilde{L}$ for the action of L on $\mathrm{so}(3)^*$ contains π. Hence the persisting solutions are rotating choreographies. Part d) follows from Theorem 3.17 c). ∎

4.5 Rotating Eight solutions of the three-body system and their bifurcations

In this section we apply the persistence result Corollary 4.3 to the Figure Eight solution of the three-body system. We reprove the existence of three types of rotating Eights. These existence results were first obtained by Chenciner et al [4]. Numerically we find a relative period doubling bifurcation along the branch of the planar (type III) rotating choreographies and compute the branch of rotating choreographies bifurcating it.

4.5.1 Three families of rotating Eights

The Figure Eight is a choreography of the planar 3-identical-body system (4.2), $N = 3$. However we regard the planar system as being embedded in the three-body system in $\mathbb{R}^3$ and consider the persistence of the Figure Eight to (in general non-planar) relative periodic orbits.

Let $\{e_1, e_2, e_3\}$ be a fixed orthogonal set of axes in $\mathbb{R}^3$ and assume that the Eight lies in the plane perpendicular to e_3 aligned along the e_2 axis with both e_2 axis and e_1 axis as symmetry axis. As before, for $i = 1, 2, 3$ let κ_i denote the (time-preserving) reflection with reflection axis e_i. The purely spatial symmetry group of the Figure Eight choreography is the group

$$K = \mathbb{Z}_2 = \langle \kappa_3 \rangle$$

generated by κ_3, a reflection about the (x_1, x_2)-plane containing the Figure Eight. The spatio-temporal symmetry group of the Eight is the group

$$L = \mathbb{Z}_2 \times \mathbb{Z}_6 = \langle \kappa_3, \kappa_1(231) \rangle.$$

The drift symmetry $\alpha := \kappa_1(231)$ is a reflection in the $\{e_1, e_2\}$-plane composed with a cyclic permutation of the bodies and has order $\ell = 6$. It has the following matrix form in the planar reduced phase space coordinates $(q_1, q_2, p_1, p_2) \in \mathbb{R}^8$:

$$\alpha := \begin{pmatrix} \alpha_q & 0 \\ 0 & \alpha_p \end{pmatrix}, \quad \alpha_q = \alpha_p = \begin{pmatrix} -\kappa & -\kappa \\ \kappa & 0 \end{pmatrix}, \quad \text{where } \kappa = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

There is a one-parameter family of Figure Eight solutions with spatio-temporal symmetry L close to the original Figure Eight, parametrized by energy. Since the three-body problem is invariant under the scaling

$$x(t) = (q(t), p(t)) \to (cq(c^{-3/2}t), c^{-1/2}p(c^{-3/2}t)), \tag{4.4}$$

the Figure Eight solutions of this one-parameter family are just rescalings of the original Figure Eight. To obtain qualitatively new solutions we need to continue with respect to other parameters, e.g. momentum.

Since the permutation group S_3 acts trivially on momentum space $\mathbf{g}^* \cong \mathbb{R}^3$ the action of L on $\mathbf{g}^*$ reduces to the action of $\langle \kappa_3, \kappa_1 \rangle \simeq \mathbb{Z}_2 \times \mathbb{Z}_2$. The isotropy subgroups of this group with one dimensional fixed point spaces on $\mathbf{g}^*$ are

I. $\langle \kappa_1 \rangle$ lifting to the subgroup $L^I = \langle \kappa_1(231) \rangle \cong \mathbb{Z}_6$ of L;

II. $\langle \kappa_1\kappa_3 \rangle$ lifting to the subgroup $L^{II} = \langle \kappa_1\kappa_3(231) \rangle \cong \mathbb{Z}_6$ of L;

III. $\langle \kappa_3 \rangle$ lifting to the subgroup $L^{III} = \langle \kappa_3, (312) \rangle \cong \mathbb{Z}_3 \times \mathbb{Z}_2$ of L.

The initial data for the Figure Eight solution are (up to 5 digits of accuracy, see [6])

$$q_1 = -q_2 = (0.97000, -0.24308, 0), \quad p_1 = p_2 = (0.46620, 0.43237, 0), \quad T = 6.3259.$$

We numerically computed the following eigenvalues of the derivative of the reduced Poincaré map in the planar Figure Eight solution:

$$\lambda_{1,2} = 1.00, \quad \lambda_{3,4} = -1.00, \quad \lambda_{5,6} = -0.508 \pm \mathrm{i}0.862, \quad \lambda_{7,8} = 0.210 \pm \mathrm{i}0.978.$$

Hence the Figure Eight solution is non-degenerate in the sense of Definition 3.11. It is also non-degenerate when considered as periodic orbit with symmetry group L^I, L^{II} and L^{III} respectively. Hence we verified numerically that the Figure Eight solution satisfies the non-degeneracy assumption of Corollary 4.3 (note that $\lambda_{5,6} \approx \mathrm{e}^{\pm \mathrm{i}2\pi/3}$ so that the Figure Eight is almost degenerate when considered as T-periodic orbit with trivial spatio-temporal symmetry.) Therefore by Corollary 4.3 there exist two-parameter families of rotating choreographies with spatio-temporal symmetry groups isomorphic to the groups listed above. We describe each in turn (see also [4]):

I. The angular velocity vector ω^I of the type I rotating Eight is parallel to the e_1 axis and thus the Eight rotates around its longer axis. The time-preserving reflection in the $\{e_1, e_2\}$-plane is preserved, but the reflection symmetry in the plane of the original Eight is broken. Thus the Eights in the rotating frame are no longer planar. The drift symmetry in the rotating frame $\alpha^I = \kappa_1(231)$ has order $\ell^I = 6$ and the relative periods $\tau^I(E,\nu)$ of the bifurcating RPOs $\mathcal{P}^I(E,\nu)$ are close to the relative period of the original Figure Eight, $\tau^I(0,0) = \bar{\tau}$.

II. The angular velocity vector ω^{II} is parallel to the e_2 axis and thus the bifurcating Eights rotate around their smaller axis. *All* the reflectional symmetries are broken, but the 180 degree rotational symmetry $R_2 := \kappa_1\kappa_3$ about the e_2 axis is preserved. Again the rotating Eight is fully three dimensional. The drift symmetry in the rotating frame $\alpha^{II} = \kappa_1\kappa_3(231)$ has order $\ell^{II} = 6$ and the relative periods $\tau^{II}(E,\nu)$ of the bifurcating RPOs $\mathcal{P}^{II}(E,\nu)$ are close to the relative period of the original Figure Eight, $\tau^{II}(0,0) = \bar{\tau}$.

III. The angular velocity vector $\omega^{III} || e_3$ is perpendicular to the (x_1, x_2)-plane containing the original Eight and the rotating Eights also continue to lie in that plane. In the rotating coordinates the trajectories look like eights, but with less symmetry: the time-preserving reflection κ_1 is broken. The drift symmetry in the rotating frame $\alpha^{III} = (312)$ has order $\ell^{III} = 3$ and the relative period $\tau^{III}(E,\nu)$ of the family of bifurcating RPOs $\mathcal{P}^{III}(E,\nu)$ has doubled at the bifurcation point: $\tau^{III}(0,0) = 2\bar{\tau}$.

So, there are three families of RPOs which take the form of eights rotating about 3 perpendicular axes. Moreover, by Corollary 4.3, each of these families is locally unique, i.e., any RPO close to the Figure Eight with the symmetry data as prescribed for the families above, will belong to one of those families. These three families of rotating Eights have been computed numerically using the methods described before in the code SYMPERCON [32] and are illustrated in the corotating frame in Figure 1.

Remarks 4.4

a) In Remark 4.1 we mentioned that the N-body system (4.2) also has time-reversing symmetries. A time-reversing symmetry $\bar{\rho} = \rho\gamma$, $\gamma \in \Gamma$, of (4.2) is called a time-reversing symmetry of an RPO $\bar{\mathcal{P}}$ with respect to $\bar{x} = x(0) \in \bar{\mathcal{P}}$ if $\bar{\rho}\bar{x} = x(t)$ for some t. If $\bar{\rho}\bar{x} = \bar{x}$ then we say that $\bar{\rho}$ lies in the *reversing isotropy group* K_ρ of $\bar{x}$. The Figure Eight has the reversing symmetry $\bar{\rho} \in K_\rho$ given by $\bar{\rho} = \kappa_2(132)\rho$, if we choose $\bar{x} = x(0)$ such that the first particle lies on the e_1-axis, and the second and third particle have the same e_1-component, see [4, 30]. The reversing spatio-temporal symmetry L_ρ of the Figure Eight is then isomorphic to $L_\rho \simeq \mathbb{D}_6 \ltimes \mathbb{Z}_2$.

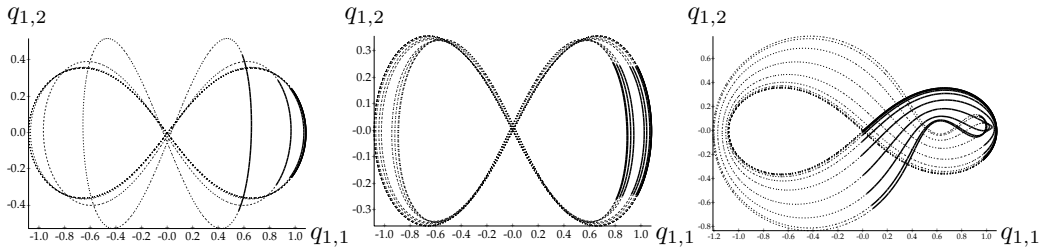

Figure 1: Trajectories of $q_1(t) = (q_{1,1}(t), q_{1,2}(t))$ of rotating Figure Eights of types I,II and III for varying angular momenta, at fixed energy $H = -1.2871$, in a corotating frame.

Reversing symmetries ρ act on momenta $\mu \in \mathbf{g}^*$ and infinitesimal symmetries $\xi \in \mathbf{g}$ as follows (see [37]):

$$\rho\mu = -(\mathrm{Ad}^*_\rho)^{-1}\mu, \quad \rho\xi = -\mathrm{Ad}_\rho\xi.$$

Theorem 3.17 and Corollary 4.3 can be extended to include time-reversing symmetries by just replacing the spatio-temporal symmetry groups of the original and bifurcating solutions with the corresponding time-reversal spatio-temporal symmetry groups. One can then check that the type I rotating Eight at angular momentum 0 has the reversing symmetry $\rho^I = \rho\kappa_2(132)$ with respect to $\bar{x}$, that the type II rotating Eight has the reversing symmetry $\rho^{II} = \rho\kappa_2\kappa_3(132)$ and that the type III rotating Eight has the reversing symmetry $\rho^{III} = \rho^I$. Hence, the reversing spatio-temporal symmetries of the three types of rotating Eights are isomorphic to

$$L^I_\rho \simeq \mathbb{D}_6, \quad L^{II}_\rho \simeq \mathbb{D}_6, \quad L^{III}_\rho \simeq \mathbb{Z}_2 \times \mathbb{D}_3.$$

Chenciner et al [4] use these reversing symmetries to prove the existence of the type I, type II and type III rotating Eights.

b) Chenciner et al [4] continued the three families of rotating Eights numerically with respect to their rotation frequency fixing the relative period, exploiting reversing symmetries and using a finite difference scheme. We continue in angular momentum, fixing the energy. They verified numerically that the parametrization by energy/momentum and relative period/velocity are equivalent for rotating Eights near the Figure Eight by checking that the corresponding Jordan block of the linearization of the Figure Eight does not vanish, cf. Section 3.5.2. They also numerically checked the nondegeneracy of the Figure Eight.

c) Galán et al [15] also continue choreographies of the three-body system, but they restrict attention to continuation of periodic orbits of fixed period with respect to an external parameter (the mass ratio of two bodies). They do not fix the centre of mass at 0 as we do. Without this reduction the three-body problem has a 6-dimensional symmetry group $\Gamma = \mathrm{SO}(3) \ltimes \mathbb{R}^3$. They then apply the numerical methods described in Remark 3.26 with $g = \dim \Gamma = 6$.

4.5.2 Relative period doubling of planar rotating Eights

The third picture of Figure 1 shows the planar (type III) family of RPOs bifurcating from the "Eight" for angular momentum near 0. For larger angular momentum this family of RPOs comes close to a collision, see Figure 2. In order to continue the family near the collision we increased the size of the RPOs thus decreasing the energy using the scaling symmetry (4.4) of the three body problem. Figure 2 shows the trajectory of the first component $p_{1,1}$ of the momentum p_1 of the first body over the first component $q_{1,1}$ of the position q_1 of the first body

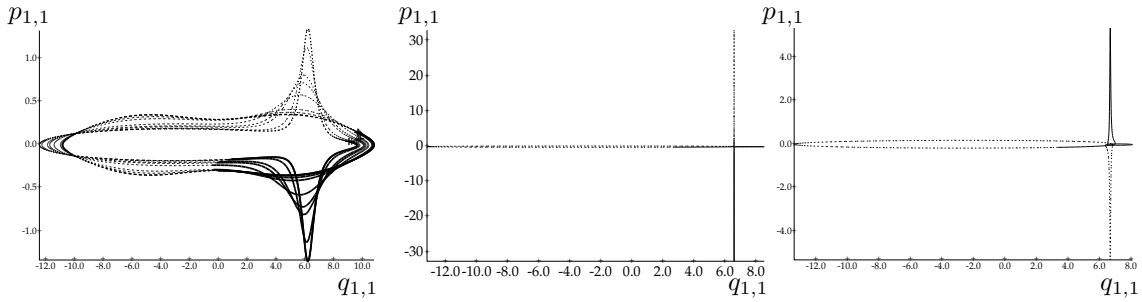

Figure 2: RPOs of type III close to collision, at fixed energy $H = -0.12871$, in a corotating frame, see text.

of the RPOs for different values of the angular momentum. In the first picture the momentum ranges between $\mathbf{J} = 0$ and $\mathbf{J} = -1.3079$, the RPO in the second picture is closest to collision and has momentum $\mathbf{J} = -2.2136$, the RPO in the third picture, after the nearby collision, has momentum $\mathbf{J} = -2.5674$. On the whole branch the condition of the condensed matrix M_c^E from (2.37) is never below 10^7, but the Jacobian J of the multiple shooting equation $F^E = 0$ from (2.35) is well-conditioned. This shows how well the iterative refinement technique, see Remark 2.13, stabilizes the block Gaussian elimination.

After coming very close to a collision SYMPERCON detected a relative period doubling bifurcation of this family of RPOs at energy $H = -0.12871$ and momentum $\mathbf{J} = -6.6383$, see the left picture on the first row of Figure 3. This is an example of a generic bifurcation of RPOs. The drift symmetry $\tilde{\alpha}$ of the bifurcating family of RPOs in the corotating frame is given by $\tilde{\alpha} = (\alpha^{III})^2 = (231)$ and so the bifurcating RPOs are rotating choreographies. The initial values, the period T in the corotating frame and the rotation frequency ω of the bifurcation point as computed by SYMPERCON are

$$\begin{aligned} &q_1 = (1.4822, -0.34773), \quad q_2 = (-9.1785, 5.8329), \\ &p_1 = (0.028466, 0.11164), \quad p_2 = (0.15917, 0.23685), \\ &T = 325.86, \quad \omega = -0.00049047. \end{aligned}$$

The Floquet eigenvalues are

$$\lambda_{1,2,3,4} = 1, \quad \lambda_{5,6} = -1, \quad \lambda_7 = 20.2, \quad \lambda_8 = 0.0496.$$

Note that a similarly looking choreography, but with vanishing drift velocity and different period, has been found by Simó [33, left picture in row 2 of Figure 14].

The right picture in the first row of Figure 3 shows the bifurcating rotating choreography at energy $H = -0.12871$ and momentum $\mathbf{J} = -6.6347$. The initial values, the period in the corotating frame and the rotation frequency of this rotating choreography are

$$\begin{aligned} &q_1 = (1.5656, -0.15778), \quad q_2 = (-9.4667, 5.6475), \\ &p_1 = (0.026277, 0.10655), \quad p_2 = (0.15712, 0.23433), \\ &T = 651.80, \quad \omega = -0.00049461. \end{aligned}$$

The Floquet eigenvalues are

$$\lambda_{1,2,3,4} = 1, \quad \lambda_5 = 2.32, \quad \lambda_6 = 0.432, \quad \lambda_7 = 343, \quad \lambda_8 = 0.00291.$$

The left picture on the second row of Figure 3 shows the bifurcating solution at energy $H = -0.12871$, momentum $\mathbf{J} = -6.5733$, rotation frequency $\omega = -0.0005695$ and period $T = 653.07$

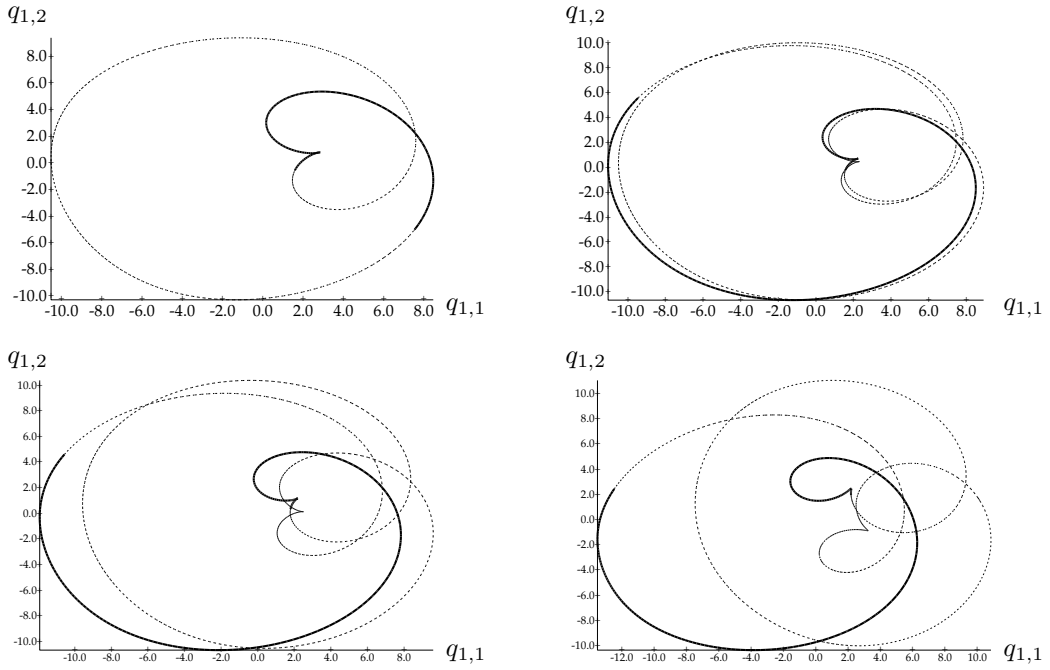

Figure 3: Rotating Eight at the relative period doubling bifurcation and bifurcating solutions, see text.

in the corotating frame; the right picture on the second row of Figure 3 shows the bifurcating solution at energy $H = -0.12871$, momentum $\mathbf{J} = -6.1795$. The initial values, the period in the corotating frame and the rotation frequency of this last RPO are

$$\begin{aligned} &q_1 = (2.1782, 2.0118), \quad q_2 = (-12.478, 2.4918), \\ &p_1 = (-0.0018436, 0.072279), \quad p_2 = (0.10945, 0.21243), \\ &T = 663.91, \quad \omega = -0.0012216. \end{aligned}$$

The Floquet eigenvalues are

$$\lambda_{1,2,3,4} = 1.00, \quad \lambda_5 = -0.531, \quad \lambda_6 = -1.88, \quad \lambda_7 = -4.67 * 10^3, \quad \lambda_8 = -0.000214.$$

In the last solution the condition of the Jacobian J of the multiple shooting equation $F = 0$ from (2.35) is computed by SYMPERCON as $\mathrm{cond}(J) = 2.73 * 10^5$, and the condition of the condensed matrix M_c^E from (2.37) is $\mathrm{cond}(M_c^E) = 1.61 * 10^{11}$. As far as we are aware this relative period doubling bifurcation of the type III family of RPOs has not been reported in the literature before. We will describe the numerical method we use for the detection and computation of this and other generic bifurcations of RPOs and will report on other bifurcations along this branch of RPOs in a forthcoming paper.

5 Conclusion and future directions

In this paper we have presented efficient algorithms for the continuation of non-degenerate symmetric periodic orbits and relative periodic orbits of Hamiltonian systems with respect to energy and (in the case of a continous symmetry group) momentum. We applied our methods to a problem from celestial mechanics. Possible other applications which we plan to work on in the future include coupled rigid bodies and robotics, underwater vehicle dynamics, dynamics of point vortices in ideal fluids and molecular dynamics.

We do not require the periodic orbits and RPOs to be reversible and hence currently we do not exploit reversing symmetries in our numerical methods. For a numerical exploitation of reversing symmetries see e.g. [4, 30, 35].

In forthcoming papers we will describe algorithms for the detection and computation of symmetry changing bifurcations of Hamiltonian RPOs building on the theoretical results [22, 23, 36] and numerical methods [38] for dissipative systems. We will then extend our methods to reversible symmetric Hamiltonian systems and design methods for the continuation of reversible RPOs and the computation of reversing symmetry breaking bifurcations. This will also require a further development of reversible equivariant bifurcation theory, see e.g. [23, 24] and the references therein for some preliminary results.

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