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Rapid and Accurate Computation of Whiskered Tori and their Manifolds Near Resonances in Periodically Perturbed Planar Circular Restricted 3-Body Problems

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Abstract When the planar circular restricted 3-body problem (RTBP) is periodically perturbed, families of unstable resonant periodic orbits break up into whiskered tori, with most tori persisting into the perturbed system. In this study, we 1) develop a quasi-Newton method which simultaneously solves for the tori and their center, stable, and unstable directions; 2) implement continuation by both perturbation as well as rotation numbers; 3) compute Fourier-Taylor parameterizations of the stable and unstable manifolds; 4) regularize the equations of motion; and 5) globalize these manifolds. Our methodology improves on efficiency and accuracy compared to prior studies, and applies to a variety of periodic perturbations. We demonstrate the tools on the planar elliptic RTBP.

1 Introduction

Numerous studies have been carried out in recent years where quasi-periodic orbits of various restricted 3-body or 4-body models have been computed and used for applications to space mission design. For instance, Farrés et al. (2017) studied periodic and quasi-periodic orbits in the phase space of the Augmented Hill 3-Body problem near the L_1 and L_2 libration points. Olikara (2016) applied collocation methods to the computation of invariant tori near L_1 and L_2 in both spatial circular restricted 3-body problem (CRTBP) as well as periodically-perturbed planar CRTBP models. And looking slightly further in the past, the book series of Gómez et al. (2001) presented many other computational methods and applications for quasi-periodic orbits near libration points. However, all of these studies, as well as almost all other prior research, use methods which require solving large-dimensional linear systems of equations at each step of the differential correction.

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Furthermore, while the quasi-periodic orbits (also known as invariant tori) are computed successfully using those methods, stability information including stable and unstable directions must be computed separately.

Another characteristic of the vast majority of prior research, including the previously mentioned studies, is that the analysis focuses on tori associated with the libration points, such as Lissajous or quasi-halo orbits. Bosanac (2018) did compute invariant tori near stable resonant periodic orbits in the planar circular restricted 3-body problem (PCRTBP), but the tori computed are stable, without stable or unstable manifolds. Unstable resonant periodic orbits and their stable and unstable manifolds are known to be important mechanisms of dynamical transport in the interior and exterior realms of the CRTBP (Koon et al. 2011), and these orbits have seen significant interest and use as a tool for trajectory design in multi-body systems. For example, out of the nine Titan-to-Titan encounters made by Cassini between July 2013 and June 2014, eight of the nine resulting transfers involved resonances (Vaquero et al. 2014). More recently, the baseline mission design for the Europa Lander mission concept made profitable use of these mechanisms for the final approach to the surface of Europa (Anderson et al. 2019). For further examples and more background on resonant orbits, see Anderson et al. (2016).

In this study, we develop efficient algorithms which enable simultaneous computation of not only unstable invariant tori, but also of their center, stable, and unstable directions (also known as bundles) in periodically perturbed PCRTBP models. Solving for bundles as well as tori actually allows us to avoid solving large linear systems, thus improving the algorithmic efficiency of our method compared to tori-only methods used in previous investigations. We apply our tools to the computation of unstable invariant tori and bundles near PCRTBP resonances, with the Jupiter-Europa planar elliptic restricted 3-body problem (PERTBP) used as the dynamical model for demonstration. Next, we use the results of the preceding step to start a recursive parameterization method (Cabré et al. 2005; Huguet et al. 2012; Haro et al. 2016) for the computation of high order Fourier-Taylor approximations of the stable and unstable manifolds of the tori. We demonstrate improvements in manifold accuracy as compared with the linear manifold approximations used in other studies. Finally, we develop a Levi-Civita regularization for the equations of motion, which is used to globalize the parameterized manifolds. We have included several proofs throughout this paper to justify our methods; these may be skipped without detriment by readers primarily interested in details of the algorithm implementation.

2 Models and Background

2.1 Planar Circular Restricted 3-body Problem

In this study, we consider periodic perturbations of the PCRTBP. The PCRTBP considers the motion of an infinitesimally small particle (thought of as a spacecraft) under the gravitational influence of two large bodies of masses m_1 and m_2, collectively referred to as the primaries. In this model, m_1 and m_2 revolve about their barycenter in a circular Keplerian orbit. Units are also normalized so that the distance between the two primaries becomes 1, $\mathcal{G}(m_1+m_2)$ becomes 1, and the primaries' period of revolution becomes 2π. We define a mass ratio $\mu = \frac{m_2}{m_1+m_2}$, and use the usual synodic, rotating non-inertial cartesian coordinate system centered at the barycenter of the primaries such that the two primaries are always on the x-axis. In the planar case we consider here, we also assume that the spacecraft moves in the same plane as the primaries. In this case, the equations of motion are Hamiltonian with form (Celletti 2010)

$$\dot{x} = \frac{\partial H_0}{\partial p_x} \quad \dot{y} = \frac{\partial H_0}{\partial p_y} \qquad \dot{p}_x = -\frac{\partial H_0}{\partial x} \quad \dot{p}_y = -\frac{\partial H_0}{\partial y} \tag{1}$$

$$H_0(x, y, p_x, p_y) = \frac{p_x^2 + p_y^2}{2} + p_x y - p_y x - \frac{1-\mu}{r_1} - \frac{\mu}{r_2} \tag{2}$$

where $r_1 = \sqrt{(x+\mu)^2 + y^2}$ is the distance from the spacecraft to m_1 and $r_2 = \sqrt{(x-1+\mu)^2 + y^2}$ is the distance to m_2.

There are two important properties of Equations (1) and (2) to note. First of all, the Hamiltonian in Eq. (2) is autonomous and is hence an integral of motion. It is related to the well-known Jacobi integral C by $H_0 = -\frac{1}{2}C$. Hence, trajectories in the PCRTBP are restricted to 3-dimensional energy submanifolds of the state space satisfying $H(x, y, p_x, p_y) = \text{constant}$. The second property to note is that the equations of motion have a time-reversal symmetry. Namely, if $(x(t), y(t), t)$ is a solution of Eq. (1) and (2) for $t > 0$, then $(x(-t), -y(-t), t)$ is a solution for $t < 0$.

2.2 Periodic Perturbations of the PCRTBP

The PCRTBP model exhibits many of the important dynamical phenomena present in multi-body celestial systems. However, there are many effects which are not included in the PCRTBP; many of these other influences on the spacecraft motion act in an approximately time-periodic manner, while preserving the Hamiltonian nature of the system. Here we will study dynamical models where one such periodic forcing effect is considered in addition to the PCRTBP. The equations of motion in this case are given by Eq. (3) along with time-periodic Hamiltonian (4)

$$\dot{x} = \frac{\partial H_\varepsilon}{\partial p_x} \quad \dot{y} = \frac{\partial H_\varepsilon}{\partial p_y} \qquad \dot{p}_x = -\frac{\partial H_\varepsilon}{\partial x} \quad \dot{p}_y = -\frac{\partial H_\varepsilon}{\partial y} \qquad \dot{\theta}_p = \Omega_p \tag{3}$$

$$H_\varepsilon(x, y, p_x, p_y, \theta_p) = H_0(x, y, p_x, p_y) + H_1(x, y, p_x, p_y, \theta_p; \varepsilon) \tag{4}$$

where $\theta_p \in \mathbb{T}$ is an angle, H_0 is the PCRTBP Hamiltonian given by Eq. (2), H_1 is the perturbation by the time-periodic effect and satisfies $H_1(x, y, p_x, p_y, \theta_p; 0) = 0$, and $\varepsilon > 0$ and Ω_p are the perturbation parameter and perturbation frequency, respectively. ε signifies the strength of the perturbation, $\varepsilon = 0$ being the unperturbed PCRTBP, and Ω_p is a known constant frequency. The perturbation from H_1 is $2\pi/\Omega_p$ periodic, with θ_p being the phase of the perturbation. Note that the Hamiltonian will no longer be constant along trajectories.

There are many different Hamiltonian periodically perturbed PCRTBP models of interest for applications. A common perturbation added to the PCRTBP is that of a third large body revolving in a circle (or approximate circle) around m_1 or m_2. Examples of these kinds of restricted 4-body models include the bicircular problem (Simó et al. 1995), the coherent quasi-bicircular problem (Andreu 1998), and the Hill restricted 4-body problem (Scheeres 1998). Another common periodically-perturbed PCRTBP model is the planar elliptic restricted 3-body problem (PERTBP), which is described in the following section.

2.3 Planar Elliptic Restricted 3-body Problem

The tools we develop in this paper are applicable to a wide variety of Hamiltonian periodic perturbations as discussed in the previous section. However, in this study, we use the PERTBP for numerical demonstration of their usage. The PERTBP has the same assumptions as the PCRTBP except that one allows m_1 and m_2 to move around their barycenter in an elliptical Keplerian orbit of eccentricity $\varepsilon > 0$. The length unit is normalized such that the semi-major axis of the m_1-m_2 orbit is 1. As the period of the primaries' orbit is 2π, we have that the perturbation frequency $\Omega_p = 1$, so we can consider $\theta_p = t$ modulo 2π.

The PERTBP model we use is essentially the same as that used by Hiday-Johnston and Howell (1994), except for a transformation from position-velocity to position-momentum coordinates and a restriction to the xy-plane. The coordinate system is again such that m_1 and m_2 are always on the x-axis with the origin at their barycenter. However, the distance between them is now time-periodic, with periapse at $t = 0$; this is different from the pulsating coordinates used by Szebehely (1967). The equations of motion are Eq. (3) with time-periodic Hamiltonian

$$H_\varepsilon(x, y, p_x, p_y, t) = \frac{p_x^2 + p_y^2}{2} + n(t)(p_x y - p_y x) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2} \tag{5}$$

where we have $n(t) = \frac{\sqrt{1-\varepsilon^2}}{(1-\varepsilon \cos E(t))^2}$, $r_1 = \sqrt{(x + \mu(1 - \varepsilon \cos E(t)))^2 + y^2}$ and $r_2 = \sqrt{(x - (1-\mu)(1 - \varepsilon \cos E(t)))^2 + y^2}$. $E(t)$ is the 2π-periodic eccentric anomaly of the elliptical m_1-m_2 orbit, and can be computed by solving the standard Kepler's equation (Bate et al. 1971). $n(t)$ is the time derivative of the m_1-m_2 true anomaly. From Eq. (3) and (5), we have $p_x = \dot{x} - n(t)y$ and $p_y = \dot{y} + n(t)x$.

2.4 Resonant Periodic Orbits

Resonant periodic orbits are PCRTBP periodic orbits which, unlike planar Lyapunov orbits, are not in the center manifold of any of the libration points. Their main characteristic is that their orbital periods are nearly rational multiples of 2π, the period of the m_1-m_2 motion (the periods become exact rational multiples of 2π as $\mu \to 0$). A resonance and its corresponding family of periodic orbits is characterized by a ratio $m : n$, $m, n \in \mathbb{Z}^+$. This notation means that in an inertial reference frame, the spacecraft makes approximately m revolutions about m_1 in the time that m_1 and m_2 revolve n times around their barycenter.

For a given resonance $m : n$ in the PCRTBP with $\mu > 0$, there typically exists one stable and one unstable resonant periodic orbit inside the submanifold $H_0(x, y, p_x, p_y) = E$, for each fixed value of E in some interval of energy values $[E_{min}, E_{max}]$ (Kumar et al. 2021a). This gives us continuous families of stable and unstable resonant periodic orbits; the periods of the orbits within a given family vary with E. The unstable resonant periodic orbits have monodromy matrix eigenvalues 1, 1, λ_s, and $\lambda_u = \lambda_s^{-1}$, where $|\lambda_s| < 1$. Thus, there are 2D stable and unstable manifolds attached to the unstable resonant periodic orbits. These manifolds serve as low-energy pathways to and from these periodic orbits. Furthermore, the manifolds of different resonances at the same energy level can intersect in the PCRTBP, giving heteroclinic connections which allow for propellant-free resonance transitions. For more details see Kumar et al. (2021a).

3 Normally Hyperbolic Invariant Manifolds and Existence of Tori

As discussed in Section 2.4, for each value of E in some interval of energy values $[E_{min}, E_{max}]$, there exists one unstable $m : n$ resonant periodic orbit in the PCRTBP. Each of these periodic orbits is diffeomorphic to a circle $\mathbb{T}$. Now, consider the union of all the unstable $m : n$ resonant periodic orbits for all values of $E \in [E_{min}, E_{max}]$. The resulting set is a 2D manifold $\varXi$ diffeomorphic to $\mathbb{T} \times [0, 1]$ in the 4D PCRTBP phase space. Furthermore, at each point of $\varXi$, there are stable and unstable directions transverse to the manifold, which come from the stable and unstable eigenvectors of the periodic orbits which make up this manifold. The phase space is 4D at each point of $\varXi$, and $\varXi$ is 2D; hence, at any point of $\varXi$, we can see that other than the two tangent vectors to the manifold, the stable and unstable directions are the only independent vectors necessary to span the phase space. This means that $\varXi$ is a normally hyperbolic invariant manifold (NHIM) of the PCRTBP flow; similar NHIMs exist for families of planar Lyapunov orbits as well (Capiński et al. 2016). A thorough discussion of NHIMs is outside the scope of this paper, but for rigorous definitions and results for flows, see Fenichel (1971).

One of the most important properties of NHIMs is that they persist under sufficiently small perturbations of the equations of motion (Fenichel 1971); as our numerical results later in this paper will demonstrate, the perturbations we study are indeed sufficiently small. However, to apply this result to our case of time-periodic perturbations, the original and perturbed systems must be defined on the same phase space. Hence, we take the PCRTBP from its original 4D phase space (x, y, p_x, p_y) to the 5D extended phase space $(x, y, p_x, p_y, \theta_p)$, $\theta_p \in \mathbb{T}$. We define $\dot{\theta}_p = \varOmega_p$ for the unperturbed PCRTBP in extended phase space, while x, y, p_x, and p_y continue to follow Equations (1) and (2). Hence, periodic orbits of period T_p from the original 4D PCRTBP phase space become 2D quasi-periodic orbits in the PCRTBP defined on the extended phase space, with one of the frequencies being $\varOmega_1 = 2\pi/T_p$ and the other being $\varOmega_p$, unless $\varOmega_1/\varOmega_p$ is rational. The NHIM $\varXi$ from the original phase space becomes the NHIM $\bar{\varXi} = \varXi \times \mathbb{T}$ in the extended phase space due to the extra angle. Hence, $\bar{\varXi}$ is diffeomorphic to $\mathbb{T}^2 \times [0, 1]$.

Now, since the PCRTBP and its NHIM have been transferred to the same extended phase space as the periodically-perturbed models, we can conclude that for $\varepsilon > 0$ sufficiently small, $\bar{\varXi}$ will persist as a NHIM $\bar{\varXi}_\varepsilon$ of the perturbed equations of motion (3) and (4). $\bar{\varXi}_\varepsilon$ will be diffeomorphic to $\bar{\varXi}$ and hence also to $\mathbb{T}^2 \times [0, 1]$. Furthermore, note that $\bar{\varXi}$ in the extended phase space PCRTBP is foliated by 2D invariant tori, since $\varXi$ was foliated by periodic orbits. From KAM theory (Capiński et al. 2016), we can expect that inside $\bar{\varXi}_\varepsilon$, the invariant tori from $\bar{\varXi}$ with sufficiently non-resonant frequencies $\varOmega_1$ and $\varOmega_p$ will also persist after perturbation with only small gaps between them. Hence, we will focus this study on these 2D tori in the periodically-perturbed PCRTBP models.

3.1 Stroboscopic Maps, NHIMs, and Invariant Circles

Any 2D invariant torus in the periodically-perturbed PCRTBP extended phase space can be parameterized as the image of a function of two angles $K_2 : \mathbb{T}^2 \to \mathbb{R}^4 \times \mathbb{T}$. A quasi-periodic trajectory $\mathbf{x}(t)$ lying on this torus can be expressed as

$$\mathbf{x}(t) = K_2(\theta, \theta_p) \qquad \theta = \theta_0 + \varOmega_1 t, \quad \theta_p = \theta_{p,0} + \varOmega_p t \tag{6}$$

where θ_0 and $\theta_{p,0}$ are determined from the initial condition $\mathbf{x}(0)$, and $\Omega_1 = 2\pi/T_p$, where T_p is the period of the PCRTBP periodic orbit associated with the torus. θ_p is the same perturbation phase angle defined in Section 2.2, so one of the two torus frequencies will be Ω_p. We can then define the stroboscopic map $F_\varepsilon : \mathbb{R}^4 \times \mathbb{T} \to \mathbb{R}^4 \times \mathbb{T}$ as the time-$2\pi/\Omega_p$ mapping of extended phase space points by the equations of motion (3) and (4) with perturbation parameter ε. We find that

$$F_\varepsilon(K_2(\theta, \theta_p)) = K_2(\theta + \omega, \theta_p), \text{ where } \omega = 2\pi\Omega_1/\Omega_p \tag{7}$$

since the angle θ_p advances by 2π in the time $2\pi/\Omega_p$ and is therefore invariant under F_ε. Hence, we can fix θ_p (for our PERTBP test case we choose $\theta_p = 0$), and then define $K(\theta) = K_2(\theta, \theta_p)$. Then, Eq. (7) becomes

$$F_\varepsilon(K(\theta)) = K(\theta + \omega) \tag{8}$$

By ignoring the last fixed θ_p component of the extended phase space and a slight abuse of notation, we can consider $F_\varepsilon : \mathbb{R}^4 \to \mathbb{R}^4$ and $K : \mathbb{T} \to \mathbb{R}^4$.

Eq. (8) implies that K parameterizes an invariant 1D torus of the map F_ε. It is significantly more computationally efficient to compute 1D invariant tori (invariant circles) K of the map F_ε in 4D phase space than 2D tori K_2 of the flow in the 5D extended phase space. The reason for this is that the reduction in the dimension of the torus helps mitigate the curse of dimensionality. Hence, from this point onwards, we will consider the map F_ε and its invariant circles and manifolds, rather than invariant objects of the continuous time flow. Similar approaches are also used by Zhang and de la Llave (2018) and Haro and Mondelo (2021).

As a final remark, the stroboscopic map allows us to use the theory of NHIMs of maps (Fenichel 1971; Hirsch et al. 1977) to understand the presence of invariant circles in periodically-perturbed PCRTBP models. In particular, note that unstable periodic orbits of the unperturbed PCRTBP are also unstable invariant circles of the map $F_{\varepsilon=0}$. Hence, the PCRTBP flow NHIM Ξ defined at the beginning of Section 3 is also a NHIM of the map $F_{\varepsilon=0}$. Just as in the case of flows, the theory shows that NHIMs of maps persist under sufficiently small perturbations of the map. Hence, for sufficiently small $\varepsilon > 0$, we can expect that Ξ will persist as a NHIM Ξ_ε of F_ε, with Ξ_ε diffeomorphic to Ξ and hence also to $\mathbb{T} \times [0, 1]$. Furthermore, since Ξ is foliated by invariant circles whose rotation numbers satisfy a twist condition, KAM theory (Capiński et al. 2016) tells us that that the invariant circles with sufficiently irrational rotation number ω persist inside Ξ_ε for $\varepsilon > 0$.

4 A Parameterization Method for Computing Invariant Tori and Bundles

In this section, we develop and implement a parameterization method for the simultaneous computation of unstable invariant tori as well as their center, stable, and unstable directions, also known as bundles, for stroboscopic maps of periodically-perturbed PCRTBP models. We present the analytical details and derivation of the method, as well as the considerations required for its discretization and numerical implementation in a computer program. The method is broadly inspired by the methods of Haro et al. (2016), except for the additional presence of a center bundle which is not considered by them and requires additional calculations. A computationally different but conceptually related method can also be found in the work of Fontich et al. (2009).

4.1 The Parameterization Method for Invariant Manifolds

The parameterization method is a general technique for the computation of many kinds of invariant objects in dynamical systems, including tori and stable and unstable manifolds. Haro et al. (2016) describe several applications. The idea is that given a map $F : \mathbb{R}^d \to \mathbb{R}^d$, if we know that there is an F-invariant object diffeomorphic to some model manifold $\mathcal{M}$, then we can solve for a function $W : \mathcal{M} \to \mathbb{R}^d$ and a diffeomorphism $f : \mathcal{M} \to \mathcal{M}$ such that the invariance equation

$$F(W(s)) = W(f(s)) \tag{9}$$

holds for all $s \in \mathcal{M}$. W is referred to as the parameterization of the invariant manifold, and f as the internal dynamics on $\mathcal{M}$. Eq. (9) means that F maps the image $W(\mathcal{M})$ into itself, so that $W(\mathcal{M})$ is the invariant object in the full space $\mathbb{R}^d$.

4.2 Equations for Parameterization Method for Tori and Bundles

For notational convenience, denote the stroboscopic map F_ε from Section 3.1 as F from now on. We assume that the rotation number $\omega = 2\pi\Omega_1/\Omega_p$ is known for the invariant circle we are trying to compute; this is the case whenever the circle comes from a PCRTBP periodic orbit of known period T_p and hence known $\Omega_1 = 2\pi/T_p$. As given in Eq. (8), we wish to find a parameterization $K : \mathbb{T} \to \mathbb{R}^4$ of the F-invariant circle satisfying the torus invariance equation

$$F(K(\theta)) = K(\theta + \omega) \tag{10}$$

This is equivalent to the framework of Section 4.1 with $\mathcal{M} = \mathbb{T}$ and $f(s) = s + \omega$. In addition, for our quasi-Newton method, we will add another equation to be solved for matrix-valued periodic functions $P(\theta)$, $\Lambda(\theta) : \mathbb{T} \to \mathbb{R}^{4\times 4}$ such that

$$DF(K(\theta))P(\theta) = P(\theta + \omega)\Lambda(\theta) \tag{11}$$

Furthermore, we mandate that $\Lambda(\theta)$ has the form

$$\Lambda(\theta) = \begin{bmatrix} 1 & T(\theta) & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \lambda_s(\theta) & 0 \\ 0 & 0 & 0 & \lambda_u(\theta) \end{bmatrix} \tag{12}$$

for some functions $T(\theta), \lambda_s(\theta), \lambda_u(\theta) : \mathbb{T} \to \mathbb{R}$ to be solved for. The form of Eq. (12) is motivated by geometric considerations that we will detail in Section 4.3.

As will be explained at the end of Section 4.5, solving simultaneously for K, P, and Λ is actually more efficient than solving for K alone; the quasi-Newton method we will present for solving Eq. (10)-(11) uses the near-diagonal form of Λ to decouple the linear system of equations we get in each differential correction step. The method will require only algebraic operations, phase shifts, and the solving of 1D equations for scalar-valued functions.

4.3 Understanding the P and Λ Matrices

In addition to their numerical utility, P and Λ have a geometric significance which will be useful when computing stable and unstable manifolds later on. Since K is contained in the 2D normally hyperbolic invariant manifold Ξ_ε defined at the end of Section (3.1), we know that there are tangent, center, stable, and unstable directions to the torus at each point $K(\theta)$. The columns of P will be these four vector bundles, with $\lambda_s(\theta)$ and $\lambda_u(\theta)$ set to the stable and unstable multipliers for the corresponding bundles. To see why, consider Eq. (11) column by column.

Let $\mathbf{v}_t(\theta), \mathbf{v}_c(\theta)$, $\mathbf{v}_s(\theta)$, and $\mathbf{v}_u(\theta)$ denote the first, second, third, and fourth columns of $P(\theta)$, respectively. Then, Equations (11) and (12) are equivalent to

$$DF(K(\theta))\mathbf{v}_t(\theta) = \mathbf{v}_t(\theta+\omega) \tag{13}$$

$$DF(K(\theta))\mathbf{v}_c(\theta) = T(\theta)DK(\theta+\omega) + \mathbf{v}_c(\theta+\omega) \tag{14}$$

$$DF(K(\theta))\mathbf{v}_s(\theta) = \lambda_s(\theta)\mathbf{v}_s(\theta+\omega) \tag{15}$$

$$DF(K(\theta))\mathbf{v}_u(\theta) = \lambda_u(\theta)\mathbf{v}_u(\theta+\omega) \tag{16}$$

First of all, note that Eq. (15)-(16) are the definition of stable and unstable bundles $\mathbf{v}_s(\theta)$ and $\mathbf{v}_u(\theta)$ and multipliers $\lambda_s(\theta)$ and $\lambda_u(\theta)$ for the torus K. Hence, the third and fourth columns of P satisfy Eq. (11) if and only if they are torus stable and unstable bundles, respectively. Also, differentiating Eq. (10) gives

$$DF(K(\theta))DK(\theta) = DK(\theta+\omega) \tag{17}$$

which shows that $\mathbf{v}_t(\theta) = DK(\theta)$ solves Eq. (13). As a result, the first column of P can be set as the torus tangent bundle $DK(\theta)$; in fact, if Eq. (11) has a solution, it is easy to show that column 1 of P *must* be $\alpha DK(\theta)$ for some $\alpha \in \mathbb{R}$.

Finally, since F is a Hamiltonian flow map and hence is symplectic, given $K(\theta)$, $\mathbf{v}_s(\theta)$, and $\mathbf{v}_u(\theta)$, we can find $\mathbf{v}_c(\theta)$ solving Eq. (14) for some function $T : \mathbb{T} \to \mathbb{R}$; we postpone the description and proof of how to compute such a $\mathbf{v}_c(\theta)$ to Section 4.8 where the method will be used. Any such $\mathbf{v}_c(\theta)$ is known as a symplectic conjugate to $DK(\theta)$, and is a center direction to the torus K (de la Llave et al. 2005). Hence, column 2 of P satisfies Eq. (11) if and only if it is a symplectic conjugate center bundle. We should note that Eq. (11) is actually underdetermined; symplectic conjugates are not unique, and we can change the scales of the stable and unstable bundles; we will take advantage of this in Section 4.7 to make Λ constant.

4.4 Summary of Steps for Quasi Newton-Method

We will now develop our quasi-Newton method for solving Eq. (10) and (11). Before presenting the details of the method, we give a brief overview. Assume we have an approximate solution (K, P, Λ) for Eq. (10)-(11). Then, we will

1. Compute $E(\theta) = F(K(\theta)) - K(\theta+\omega)$, $E_{red}(\theta) = P^{-1}(\theta+\omega)DF(K(\theta))P(\theta) - \Lambda(\theta)$
2. Solve $-P^{-1}(\theta+\omega)E(\theta) = \Lambda(\theta)\xi(\theta) - \xi(\theta+\omega)$ for $\xi : \mathbb{T} \to \mathbb{R}^4$ using Eq. (23)-(26) and set $K(\theta)$ equal to $K(\theta) + P(\theta)\xi(\theta)$ (details given in Section 4.5).
3. Set column 1 of $P(\theta)$ to $DK(\theta)$. Recompute $DF(K(\theta))$ and $E_{red}(\theta)$.
4. Solve $-E_{red}(\theta) = \Lambda(\theta)Q(\theta) - Q(\theta+\omega)\Lambda(\theta) - \Delta\Lambda(\theta)$ for $Q : \mathbb{T} \to \mathbb{R}^{4\times 4}$ and $\Delta\Lambda$ using Eq. (37)-(48). Set $P(\theta)$ equal to $P(\theta) + P(\theta)Q(\theta)$ and $\Lambda(\theta)$ equal to $\Lambda(\theta) + \Delta\Lambda(\theta)$ (details given in Section 4.6).
5. Return to step 1 and repeat correction until E and E_{red} are within tolerance.

4.5 Quasi-Newton Step for Correcting K

We seek to solve Eq. (10) and (11) for K, P, and Λ. All the entries of Λ are fixed as 0 or 1 as shown in Eq. (12) except for $T(\theta)$, $\lambda_s(\theta)$, and $\lambda_u(\theta)$. We will now derive an iterative step that, given an approximate solution (K, P, Λ) of Eq. (10) and (11), produces a much more accurate one. Define the errors

$$E(\theta) = F(K(\theta)) - K(\theta + \omega) \tag{18}$$

$$E_{red}(\theta) = P^{-1}(\theta + \omega) DF(K(\theta)) P(\theta) - \Lambda(\theta) \tag{19}$$

We then need to find corrections ΔK, ΔP, and $\Delta\Lambda$ to cancel E and E_{red}. We start with ΔK; write $\Delta K(\theta) = P(\theta)\xi(\theta)$. We will solve for $\xi : \mathbb{T} \to \mathbb{R}^4$ satisfying

$$\eta(\theta) \overset{\text{def}}{=} -P^{-1}(\theta + \omega)E(\theta) = \Lambda(\theta)\xi(\theta) - \xi(\theta + \omega) \tag{20}$$

Claim For ω sufficiently irrational and E and E_{red} sufficiently small, if ξ solves Eq. (20), then adding $\Delta K = P\xi$ to K reduces the error E quadratically.

Remark 1 We use the phrase "sufficiently irrational" when describing conditions on ω that ensure the validity of our quasi-Newton method. For those aware of KAM theory, what we mean by this is that ω must be Diophantine, as most numbers are (Huguet et al. 2012). This condition arises due to the classic small-divisors problem of KAM theory when solving cohomological equations (see Eq. (30)).

Proof Substitute $K(\theta) + \Delta K(\theta)$ into the RHS of Eq. (18). Assuming that ΔK is small enough (true if E is sufficiently small), we can expand in Taylor series to get

$$\begin{aligned} E_{new}(\theta) &= F(K(\theta) + \Delta K(\theta)) - [K(\theta + \omega) + \Delta K(\theta + \omega)] \\ &= F(K(\theta)) + DF(K(\theta))\Delta K(\theta) + O(\Delta K(\theta)^2) - [K(\theta + \omega) + \Delta K(\theta + \omega)] \\ &= E(\theta) + DF(K(\theta))\Delta K(\theta) - \Delta K(\theta + \omega) + O(\Delta K(\theta)^2) \end{aligned} \tag{21}$$

$\Delta K = P\xi$, and Eq. (19) implies $DF(K(\theta))P(\theta) = P(\theta + \omega)\,[\Lambda(\theta) + E_{red}(\theta)]$. Thus,

$$\begin{aligned} E_{new}(\theta) &= E(\theta) + DF(K(\theta))P(\theta)\xi(\theta) - P(\theta + \omega)\xi(\theta + \omega) + O(\xi(\theta)^2) \\ &= E(\theta) + P(\theta + \omega)\,[\Lambda(\theta)\xi(\theta) + E_{red}(\theta)\xi(\theta) - \xi(\theta + \omega)] + O(\xi(\theta)^2) \\ &= P(\theta + \omega)E_{red}(\theta)\xi(\theta) + O(\xi(\theta)^2) \end{aligned} \tag{22}$$

where the last line follows from Eq. (20). For ω sufficiently irrational, ξ will be similar in magnitude to E, so $E_{red}(\theta)\xi(\theta)$ will be quadratically small like $E_{red}(\theta)E(\theta)$. Hence, as long as E (and hence ξ and ΔK) are small enough that the Taylor expansion in Eq. (71) is valid, and the $O(\xi^2)$ terms of the Taylor expansion are small, the new error E_{new} will be quadratically smaller than E. □

To solve Eq. (20), let $\xi(\theta) = \begin{bmatrix}\xi_1 \ \xi_2 \ \xi_3 \ \xi_4\end{bmatrix}^T$ and $\eta_(\theta) = \begin{bmatrix}\eta_1 \ \eta_2 \ \eta_3 \ \eta_4\end{bmatrix}^T$. As Λ is nearly diagonal, we can write Eq. (20) component-wise as

$$\eta_1(\theta) - T(\theta)\xi_2(\theta) = \xi_1(\theta) - \xi_1(\theta + \omega) \tag{23}$$

$$\eta_2(\theta) = \xi_2(\theta) - \xi_2(\theta + \omega) \tag{24}$$

$$\eta_3(\theta) = \lambda_s(\theta)\xi_3(\theta) - \xi_3(\theta + \omega) \tag{25}$$

$$\eta_4(\theta) = \lambda_u(\theta)\xi_4(\theta) - \xi_4(\theta + \omega) \tag{26}$$

4.5.1 Fixed-Point Iteration: Solving for ξ_3 and ξ_4

To solve for ξ_3 and ξ_4, rewrite Equations (25) and (26) in the form

$$\xi_3(\theta) = \lambda_s(\theta-\omega)\xi_3(\theta-\omega) - \eta_3(\theta-\omega) \overset{\text{def}}{=} [A(\xi_3)](\theta) \tag{27}$$

$$\xi_4(\theta) = \lambda_u^{-1}(\theta)\,[\eta_4(\theta) + \xi_4(\theta+\omega)] \overset{\text{def}}{=} [B(\xi_4)](\theta) \tag{28}$$

We define A as a map from functions to functions, which sends any $f(\theta) : \mathbb{T} \to \mathbb{R}$ to the new function $[A(f)](\theta) = \lambda_s(\theta-\omega)f(\theta-\omega) - \eta_3(\theta-\omega)$; B is defined similarly using Eq. (28). To find ξ_3 and ξ_4, let $\xi_{3,0} = \xi_{4,0} = 0$ and iterate $\xi_{3,n+1} = A(\xi_{3,n})$ and $\xi_{4,n+1} = B(\xi_{4,n})$ repeatedly, starting at $n = 0$. The iterations will converge to the desired solutions ξ_3 and ξ_4 of Eq. (27) and (28). We now explain why.

Lemma 1 *A and B are contraction maps, and the iterations $\xi_{3,n+1} = A(\xi_{3,n})$ and $\xi_{4,n+1} = B(\xi_{4,n})$ converge exponentially fast as $n \to \infty$ to the solutions ξ_3 and ξ_4.*

Proof Note that $|\lambda_s(\theta)| < 1$ and $|\lambda_u^{-1}(\theta)| < 1$ for all $\theta \in \mathbb{T}$. Let $f_1, f_2 : \mathbb{T} \to \mathbb{R}$ be two continuous functions, and define $C = \max_{\theta\in\mathbb{T}} |\lambda_s(\theta)| < 1$. We have that

$$\begin{aligned}
&\max_{\theta\in\mathbb{T}} \|[A(f_1)](\theta) - [A(f_2)](\theta)\| \\
&\qquad = \max_{\theta\in\mathbb{T}} \|\lambda_s(\theta-\omega)f_1(\theta-\omega) - \lambda_s(\theta-\omega)f_2(\theta-\omega)\| \\
&\qquad \le C \max_{\theta\in\mathbb{T}} \|f_1(\theta-\omega) - f_2(\theta-\omega)\| = C \max_{\theta\in\mathbb{T}} \|f_1(\theta) - f_2(\theta)\|
\end{aligned} \tag{29}$$

As $C < 1$, A is a contraction map under the uniform norm; the same can be shown for B very similarly. The contraction mapping theorem (Chicone 2006) tells us that every such map has a unique fixed point; furthermore, the fixed point can be found by iterating any value in the domain of the map forwards until convergence. The solutions of Equations (27) and (28) are by definition the fixed points of contraction maps A and B. Hence, the iterations converge to ξ_3 and ξ_4. □

Remark 2 If λ_s and λ_u are constant, Fourier methods (see Section 4.5.2) can also be used to solve Eq. (25) and (26). We did not ensure constant λ_s and λ_u in our implementation of the algorithm, hence the use of fixed-point iteration instead.

4.5.2 Cohomological Equations: Solving for ξ_1 and ξ_2

We next solve Eq. (24) for ξ_2, which is then used in the LHS of Eq. (23) to solve for ξ_1. In both cases, we must solve cohomological equations of form

$$b(\theta) = a(\theta) - a(\theta+\omega) \tag{30}$$

where b is known and a is not. This can easily be solved by Fourier series; let $\hat{a}(k)$ and $\hat{b}(k)$ be the kth Fourier coefficients of a and b. Then, Eq. (30) becomes

$$\sum_{k\in\mathbb{Z}} \hat{b}(k)e^{jk\theta} = \sum_{k\in\mathbb{Z}} \hat{a}(k)e^{jk\theta} - \sum_{k\in\mathbb{Z}} \hat{a}(k)e^{jk(\theta+\omega)} = \sum_{k\in\mathbb{Z}} \hat{a}(k)(1-e^{jk\omega})e^{jk\theta} \tag{31}$$

where $j = \sqrt{-1}$. Then, for ω sufficiently irrational, setting $\hat{a}(k) = \hat{b}(k)(1-e^{jk\omega})^{-1}$ allows us to compute $a(\theta)$ except for $\hat{a}(0)$. In the $k = 0$ case, $\hat{a}(0)$ cancels out on the right hand side of Eq. (30) and can hence take any value, making the solution a non-unique. Furthermore, we observe that a necessary condition for the existence of a solution is $\hat{b}(0) = 0$. $\hat{a}(0)$ and $\hat{b}(0)$ are simply the averages of a and b on $\mathbb{T}$.

We first solve Eq. (24) for $\hat{\xi}_2(k)$, $k \neq 0$, using the Fourier series method. To set $\hat{\xi}_2(0)$, first find the average α of $\eta_1 - T \times [\xi_2 - \hat{\xi}_2(0)]$. Then, choose $\hat{\xi}_2(0) = \alpha/\hat{T}(0)$, so that the LHS of Eq. (23) has zero average when solving for ξ_1. With ξ_2 fully solved, we then solve Eq. (23) for $\hat{\xi}_1(k)$, $k \neq 0$ and arbitrarily choose $\hat{\xi}_1(0) = 0$. Finally, with all four components of ξ solved, we set $K(\theta)$ equal to $K(\theta) + P(\theta)\xi(\theta)$, concluding the K correction part of the quasi-Newton step.

In practice, when solving Eq. (24) for ξ_2, we find that the average of $\eta_2(\theta)$, the left hand side of Eq. (24), is not exactly zero; we ignore this nonzero average and solve for the $\hat{\xi}_2(k)$ anyways as described earlier. $\hat{\eta}_2(0)$ decreases to zero with each quasi-Newton step as the method converges, so we are able to solve Eq. (24) more exactly; this occurs (Fontich et al. 2009) as F is an exact symplectic map, since it is a fixed-time map of a Hamiltonian system on $\mathbb{R}^4$ (Golé 2001). Also, for those familiar with the parameterization method for invariant tori, note that the choice of $\hat{\xi}_1(0) = 0$ takes care of the translation non-uniqueness of solutions of Eq. (10) without requiring extra constraint equations.

Remark 3 There are methods of numerically solving for ΔK without using P or Λ, including single-shooting (Farrés et al. 2017) and collocation (Olikara 2016) methods. These methods effectively discretize θ on a grid of N points and solve a linearized version of Eq. (71) directly for ΔK at those θ values. This requires solving at least a $4N$ dimensional linear system at each correction step. Gaussian elimination applied to this will hence have a computational complexity of $O(N^3)$. However, by using P and the nearly diagonal Λ, we decouple the equations and avoid this large dimensional system. The complexity of our quasi-Newton method is $O(N \log N)$ (as some steps use FFT). Furthermore, our method gives us not just K, but also the bundle and Floquet matrices P and Λ.

4.6 Quasi-Newton Step for Correcting P and Λ

Using the newly computed $K(\theta)$, we set the first column of $P(\theta)$ to $DK(\theta)$, and then recompute $DF(K(\theta))$ and $E_{red}(\theta)$ using Eq. (19). Finding $\Delta P(\theta)$ and $\Delta\Lambda(\theta)$ to cancel E_{red} then follows similar methodology as ΔK. Let $\Delta P(\theta) = P(\theta)Q(\theta)$; we will solve for Q and $\Delta\Lambda : \mathbb{T} \to \mathbb{R}^{4\times 4}$ satisfying

$$-E_{red}(\theta) = \Lambda(\theta)Q(\theta) - Q(\theta+\omega)\Lambda(\theta) - \Delta\Lambda(\theta) \tag{32}$$

Claim For ω sufficiently irrational and E_{red} sufficiently small, if Q and $\Delta\Lambda$ solve Eq. (32), then adding $\Delta P = PQ$ to P and $\Delta\Lambda$ to Λ reduces E_{red} quadratically.

Proof Substitute $P + PQ$ and $\Lambda + \Delta\Lambda$ into Eq. (11) to define

$$\begin{aligned}\mathcal{E}(\theta) = {} & DF(K(\theta))[P(\theta) + P(\theta)Q(\theta)] \\ & - [P(\theta+\omega) + P(\theta+\omega)Q(\theta+\omega)][\Lambda(\theta) + \Delta\Lambda(\theta)]\end{aligned} \tag{33}$$

Using $E_{red}(\theta) = P^{-1}(\theta+\omega)DF(K(\theta))P(\theta) - \Lambda(\theta)$, we then find that

$$\begin{aligned}
P(\theta+\omega)^{-1}\mathcal{E}(\theta) &= E_{red}(\theta) + P(\theta+\omega)^{-1}DF(K(\theta))P(\theta)Q(\theta) \\
&\qquad - Q(\theta+\omega)[\Lambda(\theta)+\Delta\Lambda(\theta)] - \Delta\Lambda(\theta) \\
&= E_{red}(\theta) + [\Lambda(\theta)+E_{red}(\theta)]Q(\theta) - Q(\theta+\omega)[\Lambda(\theta)+\Delta\Lambda(\theta)] - \Delta\Lambda(\theta) \\
&= E_{red}(\theta)Q(\theta) - Q(\theta+\omega)\Delta\Lambda(\theta)
\end{aligned} \tag{34}$$

where the last line follows due to Eq. (32). Evaluating Eq. (19) with $P + PQ$ and $\Lambda + \Delta\Lambda$ in place of P and Λ and denoting the result as $E_{red,new}$, we have

$$\begin{aligned}
E_{red,new}(\theta) &= [P(\theta+\omega) + P(\theta+\omega)Q(\theta+\omega)]^{-1}\mathcal{E}(\theta) \\
&= [I + Q(\theta+\omega)]^{-1}P(\theta+\omega)^{-1}\mathcal{E}(\theta) \\
&= [I + Q(\theta+\omega)]^{-1}[E_{red}(\theta)Q(\theta) - Q(\theta+\omega)\Delta\Lambda(\theta)]
\end{aligned} \tag{35}$$

Now, for ω sufficiently irrational, Q and $\Delta\Lambda$ will be similar in magnitude to E_{red}. Hence, if E_{red} is small, then $E_{red,new}$ will be quadratically smaller like E_{red}^2. $\square$

Since Λ is nearly diagonal, the equations for the different entries of Q and $\Delta\Lambda$ following from Eq. (32) are almost completely decoupled from each other. Write

$$\begin{gathered}
E_{red}(\theta) = \begin{bmatrix} E_{LL}(\theta) & E_{LC}(\theta) & E_{LS}(\theta) & E_{LU}(\theta) \\ E_{CL}(\theta) & E_{CC}(\theta) & E_{CS}(\theta) & E_{CU}(\theta) \\ E_{SL}(\theta) & E_{SC}(\theta) & E_{SS}(\theta) & E_{SU}(\theta) \\ E_{UL}(\theta) & E_{UC}(\theta) & E_{US}(\theta) & E_{UU}(\theta) \end{bmatrix} \\
Q(\theta) = \begin{bmatrix} 0 & Q_{LC}(\theta) & Q_{LS}(\theta) & Q_{LU}(\theta) \\ 0 & Q_{CC}(\theta) & Q_{CS}(\theta) & Q_{CU}(\theta) \\ 0 & Q_{SC}(\theta) & Q_{SS}(\theta) & Q_{SU}(\theta) \\ 0 & Q_{UC}(\theta) & Q_{US}(\theta) & Q_{UU}(\theta) \end{bmatrix} \quad \Delta\Lambda(\theta) = \begin{bmatrix} 0 & \Delta T(\theta) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \Delta\lambda_s(\theta) & 0 \\ 0 & 0 & 0 & \Delta\lambda_u(\theta) \end{bmatrix}
\end{gathered} \tag{36}$$

As the first column of $P(\theta)$ is fixed to be $DK(\theta)$, we fix the first column of $Q(\theta)$ to be zero so that the first column of ΔP is zero as well. We can then write columns 2-4 of Eq. (32) entry by entry to get 12 scalar equations

$$-E_{LC}(\theta) - T(\theta)Q_{CC}(\theta) = Q_{LC}(\theta) - Q_{LC}(\theta+\omega) - \Delta T(\theta) \tag{37}$$

$$-E_{LS}(\theta) - T(\theta)Q_{CS}(\theta) = Q_{LS}(\theta) - \lambda_s(\theta)Q_{LS}(\theta+\omega) \tag{38}$$

$$-E_{LU}(\theta) - T(\theta)Q_{CU}(\theta) = Q_{LU}(\theta) - \lambda_u(\theta)Q_{LU}(\theta+\omega) \tag{39}$$

$$-E_{CC}(\theta) = Q_{CC}(\theta) - Q_{CC}(\theta+\omega) \tag{40}$$

$$-E_{CS}(\theta) = Q_{CS}(\theta) - \lambda_s(\theta)Q_{CS}(\theta+\omega) \tag{41}$$

$$-E_{CU}(\theta) = Q_{CU}(\theta) - \lambda_u(\theta)Q_{CU}(\theta+\omega) \tag{42}$$

$$-E_{SC}(\theta) = \lambda_s(\theta)Q_{SC}(\theta) - Q_{SC}(\theta+\omega) \tag{43}$$

$$-E_{SS}(\theta) = \lambda_s(\theta)Q_{SS}(\theta) - \lambda_s(\theta)Q_{SS}(\theta+\omega) - \Delta\lambda_s(\theta) \tag{44}$$

$$-E_{SU}(\theta) = \lambda_s(\theta)Q_{SU}(\theta) - \lambda_u(\theta)Q_{SU}(\theta+\omega) \tag{45}$$

$$-E_{UC}(\theta) = \lambda_u(\theta)Q_{UC}(\theta) - Q_{UC}(\theta+\omega) \tag{46}$$

$$-E_{US}(\theta) = \lambda_u(\theta)Q_{US}(\theta) - \lambda_s(\theta)Q_{US}(\theta+\omega) \tag{47}$$

$$-E_{UU}(\theta) = \lambda_u(\theta)Q_{UU}(\theta) - \lambda_u(\theta)Q_{UU}(\theta+\omega) - \Delta\lambda_u(\theta) \tag{48}$$

First, we solve Equations (41), (42), (43), (45), (46), and (47), followed by Eq. (38) and (39) (after back substitution), using the exact same method that was used to solve Eq. (25) and (26); rearrange each equation so that its solution is the fixed point of an appropriately defined contraction map, which is then iterated to convergence. Such maps always multiply their input by either λ_s or λ_u^{-1}, or both. Eq. (40) is solved using the Fourier series method which was described in Section 4.5.2; we arbitrarily choose the average of the solution $\hat{Q}_{CC}(0) = 0$. We ignore the nonzero average of E_{CC}, which goes to zero as the quasi-Newton method converges due to F being exact symplectic. Finally, the solutions to Eq. (37), (44), and (48) are non-unique; we choose $Q_{LC} = Q_{SS} = Q_{UU} = 0$, so that we have $\Delta T(\theta) = E_{LC}(\theta) + T(\theta)Q_{CC}(\theta)$, $\Delta\lambda_s(\theta) = E_{SS}(\theta)$, and $\Delta\lambda_u(\theta) = E_{UU}(\theta)$.

Once Q and $\Delta\Lambda$ are known, we set $P(\theta)$ equal to $P(\theta) + P(\theta)Q(\theta)$, $\Lambda(\theta)$ equal to $\Lambda(\theta) + \Delta\Lambda(\theta)$, and then recompute $E(\theta)$ and $E_{red}(\theta)$ using Eq. (18) and (19). Finally, we go back to the quasi-Newton step for correcting the circle parameterization $K(\theta)$ and repeat the entire method until E and E_{red} are within tolerance.

Remark 4 If T, λ_s, and λ_u are constant, we can choose the non-unique solutions of Eq. (37), (44), and (48) such that this property is preserved. In particular, choose ΔT, $\Delta\lambda_s$, and $\Delta\lambda_u$ as the (constant) averages of E_{LC}, E_{SS} and E_{UU}, respectively, and solve for Q_{LC}, Q_{SS}, and Q_{UU} using the Fourier methods of Section 4.5.2.

4.7 Modifying P for Constant Λ

Let K, P, and Λ be a solution to Eq. (10) and Eq. (11). For purposes of numerical stability as well as stable/unstable manifold computation (see Section 5), it can be useful to modify the second, third, and fourth columns of P in such a way that $\Lambda = P^{-1}(\theta+\omega)DF(K(\theta))P(\theta)$ becomes a constant matrix of the form in Eq. (12), i.e. $T(\theta)$, $\lambda_s(\theta)$, and $\lambda_u(\theta)$ become constant. For columns 3 and 4 of P, the stable and unstable bundles $\mathbf{v}_s(\theta)$ and $\mathbf{v}_u(\theta)$, respectively, just a simple rescaling is needed. Let $\bar{\lambda}_s, \bar{\lambda}_u \in \mathbb{R}$ and $a_s, a_u : \mathbb{T} \to \mathbb{R}$ be the solutions to

$$\log(\lambda_s(\theta)) - \log(\bar{\lambda}_s) = \log(a_s(\theta+\omega)) - \log(a_s(\theta)) \tag{49}$$

$$\log(\lambda_u(\theta)) - \log(\bar{\lambda}_u) = \log(a_u(\theta+\omega)) - \log(a_u(\theta)) \tag{50}$$

We choose $\bar{\lambda}_s = \exp\left[\frac{1}{2\pi}\int_0^{2\pi} \log(\lambda_s(\theta))\, d\theta\right]$ so the LHS of Eq. (49) has zero average. Letting $u(\theta) = \log(a_s(\theta))$, Eq. (49) becomes a cohomological equation of form Eq. (30) which can be solved for u by the Fourier series method; we choose $\hat{u}(0) = 0$. This gives $a_s(\theta) = e^{u(\theta)}$. We can solve Eq. (50) for $a_u(\theta)$ in the exact same manner. Finally, one can replace columns 3 and 4 of P by $a_s(\theta)\mathbf{v}_s(\theta)$ and $a_u(\theta)\mathbf{v}_u(\theta)$, and replace $\lambda_s(\theta)$ and $\lambda_u(\theta)$ in Λ by $\bar{\lambda}_s$ and $\bar{\lambda}_u$. We prove that this works now.

Lemma 2 *If* $\mathbf{v}_s(\theta)$ *and* $\mathbf{v}_u(\theta)$ *satisfy Eq.* (15)-(16)*, and* $a_s(\theta)$ *and* $a_u(\theta)$ *satisfy Eq.* (49)-(50)*, then* $\mathbf{v}_{s,new}(\theta) = a_s(\theta)\mathbf{v}_s(\theta)$ *and* $\mathbf{v}_{u,new}(\theta) = a_u(\theta)\mathbf{v}_u(\theta)$ *satisfy*

$$DF(K(\theta))\mathbf{v}_{s,new}(\theta) = \bar{\lambda}_s\mathbf{v}_{s,new}(\theta+\omega) \tag{51}$$

$$DF(K(\theta))\mathbf{v}_{u,new}(\theta) = \bar{\lambda}_u\mathbf{v}_{u,new}(\theta+\omega) \tag{52}$$

Proof We prove the result for $\mathbf{v}_{s,new}$; the case of $\mathbf{v}_{u,new}$ can be proven in the exact same manner. Since $\mathbf{v}_s(\theta)$ satisfies Eq. (15), we have

$$\begin{aligned} DF(K(\theta))\mathbf{v}_{s,new}(\theta) &= DF(K(\theta))a_s(\theta)\mathbf{v}_s(\theta) = a_s(\theta)\lambda_s(\theta)\mathbf{v}_s(\theta+\omega) \\ &= a_s(\theta+\omega)\bar{\lambda}_s\mathbf{v}_s(\theta+\omega) = \bar{\lambda}_s\mathbf{v}_{s,new}(\theta+\omega) \end{aligned} \tag{53}$$

where $a_s(\theta)\lambda_s(\theta) = a_s(\theta+\omega)\bar{\lambda}_s$ follows from exponentiating Eq. (49). □

We can also modify the second column of P, the symplectic conjugate center direction $\mathbf{v}_c(\theta)$, to make $T(\theta)$ constant. This is possible because as mentioned in Section 4.3, the symplectic conjugate is not unique; given $a : \mathbb{T} \to \mathbb{R}$ and $\mathbf{v}_c(\theta)$ satisfying Eq. (14), the function $\mathbf{v}_c(\theta)+a(\theta)DK(\theta)$ also solves Eq. (14) except with a change in $T(\theta)$ (which was anyways arbitrary). Hence, we choose $a(\theta)$ which kills all variation of $T(\theta)$ about its average $\hat{T}(0)$. The equation for this is:

$$-\left(T(\theta) - \hat{T}(0)\right) = a(\theta) - a(\theta+\omega) \tag{54}$$

which can be solved using the Fourier series method given for Eq. (30). Then, one simply adds $a(\theta)DK(\theta)$ to column 2 of P and replaces $T(\theta)$ with $\hat{T}(0)$ in Λ. Note that the LHS of Eq. (54) has average zero, so a solution $a(\theta)$ can be found.

Lemma 3 *If $\mathbf{v}_c(\theta)$ and $a(\theta)$ satisfy Eq.* (14) *and* (54)*, respectively, then the function $\mathbf{v}_{c,new}(\theta) = \mathbf{v}_c(\theta) + a(\theta)DK(\theta)$ is also a symplectic conjugate and satisfies*

$$DF(K(\theta))\mathbf{v}_{c,new}(\theta) = \hat{T}(0)DK(\theta+\omega) + \mathbf{v}_{c,new}(\theta+\omega) \tag{55}$$

Proof Since $\mathbf{v}_c(\theta)$ satisfies Eq. (14) and $DK(\theta)$ satisfies Eq. (17), we have

$$\begin{aligned} DF(K(\theta))\mathbf{v}_{c,new}(\theta) &= DF(K(\theta))\left[\mathbf{v}_c(\theta) + a(\theta)DK(\theta)\right] \\ &= \left[T(\theta) + a(\theta)\right] DK(\theta+\omega) + \mathbf{v}_c(\theta+\omega) \\ &= \left[\hat{T}(0) + a(\theta+\omega)\right] DK(\theta+\omega) + \mathbf{v}_c(\theta+\omega) \\ &= \hat{T}(0)DK(\theta+\omega) + \mathbf{v}_{c,new}(\theta+\omega) \end{aligned} \tag{56}$$

where the relation $T(\theta) + a(\theta) = \hat{T}(0) + a(\theta+\omega)$ follows from Eq. (54). □

4.8 Initialization for Continuation by ε

To compute invariant circles and bundles of stroboscopic maps in periodically-perturbed PCRTBP models with some desired perturbation parameter $\varepsilon_f > 0$, we start from periodic orbits and their bundles in the unperturbed PCRTBP ($\varepsilon = 0$) and continue by ε until the torus and bundles for $\varepsilon = \varepsilon_f$ are found. Our quasi-Newton method-based continuation follows the standard procedure; choose a number of continuation steps n, take an invariant circle and bundles from the $\varepsilon = 0$ system, and use them as an initial guess for the quasi-Newton method to solve for the circle and bundles in the $\varepsilon = \varepsilon_f/n$ system. Similarly, for $i = 0, \ldots, n-1$, use the solution from the $\varepsilon_f i/n$ system as an initial guess for the solution in the $\varepsilon_f(i+1)/n$ system. Once $i = n-1$, we have the torus and bundles for $\varepsilon = \varepsilon_f$. We need to find the $\varepsilon = 0$ solution to initialize the continuation, however.

To get $K(\theta)$, $P(\theta)$, and $\Lambda(\theta)$ solving Eq. (10) and (11) for the $\varepsilon = 0$ PCRTBP case, one needs to first choose a periodic orbit which is to be continued (recall that PCRTBP periodic orbits are also invariant circles of the stroboscopic map $F = F_{\varepsilon=0}$, unless the orbit period is resonant with $2\pi/\Omega_p$). From this periodic orbit, we get its period T_p and hence the rotation number $\omega = 4\pi^2/(T_p\Omega_p)$, as well as a point $\mathbf{x}_0$ lying on the orbit. Let $\phi(\mathbf{x}, t)$ denote the time-t map of the point $\mathbf{x} \in \mathbb{R}^4$ by the PCRTBP equations of motion. Then, we can take $K(\theta) = \phi(\mathbf{x}_0, T_p\frac{\theta}{2\pi})$ if the periodic orbit monodromy matrix stable and unstable eigenvalues are positive. If they are negative, though, a "double covering" trick needs be used so that $P(\theta)$ can be continuously defined. For this, set $K(\theta) = \phi(\mathbf{x}_0, 2T_p\frac{\theta}{2\pi})$ and $\omega = 2\pi^2/(T_p\Omega_p)$ so that K sweeps over the periodic orbit twice as θ goes from 0 to 2π. In either case, it is easy to verify that $K(\theta)$ satisfies Eq. (10).

Next, set the first column of $P(\theta)$ to be $DK(\theta)$, and set the third and fourth columns of $P(\theta)$ as the stable and unstable unit eigenvectors of the periodic orbit monodromy matrix at the point $K(\theta)$. Denote these stable and unstable eigenvectors as $\mathbf{v}_s(\theta)$ and $\mathbf{v}_u(\theta)$, respectively. One needs to make sure that the directions of $\mathbf{v}_s(\theta)$ and $\mathbf{v}_u(\theta)$ at each point $K(\theta)$ are chosen such that they are continuously oriented functions of θ; this is always possible if K is defined as previously described. Finally, finding the second column of P requires some extra calculations.

As mentioned in Section 4.3, the second column of P represents the symplectic conjugate direction to $DK(\theta)$ and is part of the center bundle. The first step in its computation is to compute $\lambda_s(\theta)$ and $\lambda_u(\theta) : \mathbb{T} \to \mathbb{R}$ such that

$$DF(K(\theta))\mathbf{v}_s(\theta) = \lambda_s(\theta)\mathbf{v}_s(\theta + \omega) \tag{57}$$

$$DF(K(\theta))\mathbf{v}_u(\theta) = \lambda_u(\theta)\mathbf{v}_u(\theta + \omega) \tag{58}$$

which can be done since $DF(K(\theta))$ maps the stable and unstable bundles into themselves. Next, find functions $A(\theta), B(\theta), C(\theta)$, and $D(\theta) : \mathbb{T} \to \mathbb{R}$ such that

$$\begin{aligned} DF(K(\theta))\frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} = A(\theta)DK(\theta + \omega) + B(\theta)\frac{J^{-1}DK(\theta + \omega)}{\|DK(\theta + \omega)\|^2} \\ + C(\theta)\mathbf{v}_s(\theta + \omega) + D(\theta)\mathbf{v}_u(\theta + \omega) \end{aligned} \tag{59}$$

where $J = \begin{bmatrix} 0_{2\times2} & I_{2\times2} \\ -I_{2\times2} & 0_{2\times2} \end{bmatrix}$ is the 4×4 matrix of the symplectic form in the usual Euclidean metric on $\mathbb{R}^4$. All the quantities in (59) are known except for A, B, C, and D, which can hence be solved for as a system of linear equations. One will find that $B(\theta) = 1$; this occurs as a result of symplectic geometric considerations (see Eq. (68)). After this, we solve for functions $f_1(\theta), f_2(\theta) : \mathbb{T} \to \mathbb{R}$ such that

$$C(\theta) = f_1(\theta + \omega) - \lambda_s(\theta)f_1(\theta) \tag{60}$$

$$D(\theta) = f_2(\theta + \omega) - \lambda_u(\theta)f_2(\theta) \tag{61}$$

which can be done using the same contraction map iteration method used to solve Equations (25) and (26) in Section 4.5.1. Finally, we can express the second column of $P(\theta)$, the symplectic conjugate direction $\mathbf{v}_c(\theta)$, as

$$\mathbf{v}_c(\theta) = \frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} + f_1(\theta)\mathbf{v}_s(\theta) + f_2(\theta)\mathbf{v}_u(\theta) \tag{62}$$

With $P(\theta)$ known, to find Λ one can simply use $\Lambda(\theta) = P^{-1}(\theta+\omega)DF(K(\theta))P(\theta)$, after which we can start the continuation. As long as the previous steps were followed correctly, Λ will be of the form given in Eq. (12). To see this, recall the discussion in Section 4.3, and note that the first, third, and fourth columns of P satisfy Equations (13), (15), and (16). Hence, we just need to show that the second column of P satisfies Eq. (14). We prove this now.

Lemma 4 *For some $T : \mathbb{T} \to \mathbb{R}$. the function $\mathbf{v}_c(\theta)$ defined in Eq.* (62) *satisfies*

$$DF(K(\theta))\mathbf{v}_c(\theta) = T(\theta)DK(\theta+\omega) + \mathbf{v}_c(\theta+\omega) \tag{63}$$

Proof Applying Eq. (62) and then Equations (57), (58), and (59), we have

$$\begin{aligned} DF(K(\theta))\mathbf{v}_c(\theta) = DF(K(\theta)) &\left(\frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} + f_1(\theta)\mathbf{v}_s(\theta) + f_2(\theta)\mathbf{v}_u(\theta) \right) \\ =& A(\theta)DK(\theta+\omega) + B(\theta)\frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2} \\ &+ \left(C(\theta) + \lambda_s(\theta)f_1(\theta)\right)\mathbf{v}_s(\theta+\omega) + \left(D(\theta) + \lambda_u(\theta)f_2(\theta)\right)\mathbf{v}_u(\theta+\omega) \end{aligned} \tag{64}$$

Recalling Equations (60) and (61), we thus have that

$$\begin{aligned} DF(K(\theta))\mathbf{v}_c(\theta) =& A(\theta)DK(\theta+\omega) + B(\theta)\frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2} \\ &+ f_1(\theta+\omega)\mathbf{v}_s(\theta+\omega) + f_2(\theta+\omega)\mathbf{v}_u(\theta+\omega) \end{aligned} \tag{65}$$

Flow maps of Hamiltonian systems are symplectic (Thirring 1992). Hence, F satisfies $\Omega(\mathbf{v}_1, \mathbf{v}_2) = \Omega(DF(K(\theta))\mathbf{v}_1, DF(K(\theta))\mathbf{v}_2)$ for all $\mathbf{v}_1$, $\mathbf{v}_2 \in \mathbb{R}^4$, where Ω is the bilinear symplectic form defined on Euclidean $\mathbb{R}^4$ as $\Omega(\mathbf{v}_1, \mathbf{v}_2) = \mathbf{v}_1^T J \mathbf{v}_2$. It is easy to see that $\Omega(\mathbf{v}_1, \mathbf{v}_1) = 0$ for any $\mathbf{v}_1 \in \mathbb{R}^4$. Furthermore, defining $L = \max_{\theta\in\mathbb{T}} |\lambda_s(\theta)| < 1$ and recalling equations (17) and (57), we have that

$$\begin{aligned} \max_{\theta\in\mathbb{T}} |\Omega(DK(\theta), \mathbf{v}_s(\theta))| &= \max_{\theta\in\mathbb{T}} |\Omega\left(DF(K(\theta))DK(\theta), DF(K(\theta))\mathbf{v}_s(\theta)\right)| \\ &= \max_{\theta\in\mathbb{T}} |\Omega\left(DK(\theta+\omega), \lambda_s(\theta)\mathbf{v}_s(\theta+\omega)\right)| \\ &= \max_{\theta\in\mathbb{T}} |\lambda_s(\theta)|\, |\Omega\left(DK(\theta+\omega), \mathbf{v}_s(\theta+\omega)\right)| \\ &\leq L \max_{\theta\in\mathbb{T}} |\Omega\left(DK(\theta+\omega), \mathbf{v}_s(\theta+\omega)\right)| = L \max_{\theta\in\mathbb{T}} |\Omega\left(DK(\theta), \mathbf{v}_s(\theta)\right)| \end{aligned} \tag{66}$$

which implies that $\max_{\theta\in\mathbb{T}} |\Omega\left(DK(\theta), \mathbf{v}_s(\theta)\right)| = 0$ since $0 < L < 1$. Thus, for all $\theta \in \mathbb{T}$, $\Omega\left(DK(\theta), \mathbf{v}_s(\theta)\right) = 0$. We can also show that $\Omega\left(DK(\theta), \mathbf{v}_u(\theta)\right) = 0$ in a very similar manner to Eq. (66). Hence, using Eq. (62) for $\mathbf{v}_c$, we find

$$\begin{aligned} \Omega(DK(\theta), \mathbf{v}_c(\theta)) &= \Omega\left(DK(\theta), \frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} + f_1(\theta)\mathbf{v}_s(\theta) + f_2(\theta)\mathbf{v}_u(\theta) \right) \\ &= \Omega\left(DK(\theta), \frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} \right) \\ &= DK(\theta)^T J \frac{J^{-1}DK(\theta)}{\|DK(\theta)\|^2} = \frac{DK(\theta)^T DK(\theta)}{\|DK(\theta)\|^2} = 1 \end{aligned} \tag{67}$$

Since F is a symplectic map, using Eq. (65) we have that

$$\begin{aligned}1 &= \Omega(DK(\theta), \mathbf{v}_c(\theta))\\ &= \Omega\left(DF(K(\theta))DK(\theta), DF(K(\theta))\mathbf{v}_c(\theta)\right)\\ &= \Omega\Bigg(DK(\theta+\omega), A(\theta)DK(\theta+\omega) + B(\theta)\frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2}\\ &\qquad\qquad + f_1(\theta+\omega)\mathbf{v}_s(\theta+\omega) + f_2(\theta+\omega)\mathbf{v}_u(\theta+\omega)\Bigg) \qquad (68)\\ &= \Omega\left(DK(\theta+\omega), B(\theta)\frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2}\right)\\ &= B(\theta)DK(\theta+\omega)^T J\frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2} = B(\theta)\end{aligned}$$

proving that $B(\theta) = 1$. Therefore, substituting this into Eq. (65) gives

$$\begin{aligned}DF(K(\theta))\mathbf{v}_c(\theta) =& A(\theta)DK(\theta+\omega) + \frac{J^{-1}DK(\theta+\omega)}{\|DK(\theta+\omega)\|^2}\\ &+ f_1(\theta+\omega)\mathbf{v}_s(\theta+\omega) + f_2(\theta+\omega)\mathbf{v}_u(\theta+\omega)\end{aligned} \tag{69}$$

Finally, we see from Eq. (62) that the last 3 terms on the RHS are precisely $\mathbf{v}_c(\theta+\omega)$. Letting $T(\theta) = A(\theta)$, we hence conclude that

$$DF(K(\theta))\mathbf{v}_c(\theta) = T(\theta)DK(\theta+\omega) + \mathbf{v}_c(\theta+\omega) \tag{70}$$

which is what we sought to prove. □

4.9 Computing Families of Tori: Continuation by ω

The continuation by ε described in Section 4.8 is carried out with ω fixed. However, in the PCRTBP, periodic orbits occur in one-parameter families, with varying rotation numbers ω under $F_{\varepsilon=0}$. The same is true of invariant circles of F_ε for $\varepsilon = \varepsilon_f > 0$ as well. To compute the family of F_{ε_f}-invariant tori corresponding to a PCRTBP periodic orbit family, one option is to continue several different periodic orbits from that family (corresponding to different ω values) by ε. However, this is inefficient, as the tori and bundles computed for $\varepsilon < \varepsilon_f$ are not of interest. Instead, it is better to first compute just one invariant circle of F_{ε_f}, along with its bundles, at some rotation number $\omega = \omega_0$ using continuation by ε. After this, one can continue the ω_0 circle/bundles by ω, with $\varepsilon = \varepsilon_f$ fixed. The continuation by ω is quite similar to the continuation by ε; given a known exact solution to Eq. (10) and (11) for $\omega = \omega_i$, $i \in \mathbb{Z}$, one uses this to form an initial guess for the quasi-Newton method to compute the torus/bundles for $\omega = \omega_{i+1} = \omega_i + \Delta\omega_i$. This recursively gives us tori for a range of ω values. The $\Delta\omega_i$ are called the continuation step sizes.

One can use the torus and bundles for $\omega = \omega_i$ directly as an initial guess for $\omega = \omega_i + \Delta\omega_i$. However, it is extremely easy to use K, P, and Λ from ω_i to compute a better initial guess for the $\omega_i + \Delta\omega_i$ torus, which aids in quasi-Newton method convergence. Assume that Λ has constant $T(\theta) = T$ (apply the procedure from Section 4.7 to P and Λ if necessary). Then, using $\mathbf{v}_c(\theta)$ to denote column 2 of P, the initial guess for the $\omega_i + \Delta\omega_i$ torus parameterization should be $K_{new}(\theta) = K(\theta) + (\Delta\omega_i/T)\mathbf{v}_c(\theta)$. We justify this now.

Claim If K, P, and Λ (with Λ constant) solve Eq. (10)-(11) for $\omega = \omega_i$, then $K_{new}(\theta) = K(\theta) + (\Delta\omega_i/T)\mathbf{v}_c(\theta)$ solves Eq. (10) for $\omega = \omega_i + \Delta\omega_i$ up to $O(\Delta\omega_i^2)$.

Proof For notational convenience, write ω and $\Delta\omega$ in place of ω_i and $\Delta\omega_i$, respectively. Then, evaluating $F(K_{new}(\theta)) - K_{new}(\theta + \omega + \Delta\omega)$, we find this equals

$$\begin{aligned}
&F\left(K(\theta) + \frac{\Delta\omega}{T}\mathbf{v}_c(\theta)\right) - \left[K(\theta + \omega + \Delta\omega) + \frac{\Delta\omega}{T}\mathbf{v}_c(\theta + \omega + \Delta\omega)\right] \\
&\quad = F(K(\theta)) + DF(K(\theta))\frac{\Delta\omega}{T}\mathbf{v}_c(\theta) + O(\Delta\omega^2) \\
&\qquad\qquad - \left[K(\theta + \omega) + \Delta\omega DK(\theta + \omega) + \frac{\Delta\omega}{T}\mathbf{v}_c(\theta + \omega) + O(\Delta\omega^2)\right] \\
&\quad = \frac{\Delta\omega}{T}\left[DF(K(\theta))\mathbf{v}_c(\theta) - T\,DK(\theta + \omega) - \mathbf{v}_c(\theta + \omega)\right] + O(\Delta\omega^2) = O(\Delta\omega^2)
\end{aligned} \tag{71}$$

where the last equality follows from Eq. (14). □

Remark 5 Using the Poincaré-Lindstedt method, it is possible to get higher order expansions in $\Delta\omega_i$ for K_{new} than the linear approximation $K(\theta) + (\Delta\omega_i/T)\mathbf{v}_c(\theta)$. This requires significant extra computations which we decided not to carry out.

There is one more difference between continuation by ω and continuation by ε. The continuation by ε uses a fixed step size ε_f/n. However, for continuation by ω, the step size $\Delta\omega_i$ must be varied due to quasi-Newton method divergence for insufficiently irrational ω. At such ω values, the PCRTBP invariant circle breaks down after the perturbation $\varepsilon = \varepsilon_f$, leading to a gap between tori at smaller and larger rotation numbers. Our continuation needs to "jump" over this gap. Suppose we have a torus and bundles for $\omega = \omega_i$, and let φ_i denote the largest of $\Delta\omega_{i-1}, \Delta\omega_{i-2}, \ldots, \Delta\omega_{i-5}$. It is natural to try $\Delta\omega_i = \varphi_i$. If the quasi-Newton method diverges for $\omega = \omega_i + \varphi_i$, however, then instead one can try $\Delta\omega_i = \varphi_i/2$; if this still does not work, try $\Delta\omega_i = \varphi_i/2^2$, and so on until we find a $\Delta\omega_i$ that works. Once we have the circle/bundles for $\omega_{i+1} = \omega_i + \Delta\omega_i$, we repeat the process.

In this procedure, it is possible for $\Delta\omega_{i+1}$ to be larger than $\Delta\omega_i$, which is what allows us to "jump" over gaps in the tori. For example, suppose that $\Delta\omega_{i-1}$ through $\Delta\omega_{i-5}$ are all equal to $\phi = \frac{1+\sqrt{5}}{2} \times 10^{-4}$, so $\varphi_i = \phi$. Then, it can happen that the quasi-Newton method diverges for $\omega = \omega_i + \phi$, but converges for $\omega = \omega_i + \phi/2 = \omega_{i+1}$, so $\Delta\omega_i = \phi/2$. However, φ_{i+1} will still equal ϕ, so we try $\Delta\omega_{i+1} = \phi$. If the quasi-Newton method converges for $\omega = \omega_{i+1} + \phi = \omega_i + 3\phi/2$, then we will have crossed the torus gap encountered earlier at $\omega = \omega_i + \phi$. This is schematically illustrated in Figure 1; we draw the tori on a projection of the 2D cylindrical NHIM Ξ_ε defined in Section 3.1 (we let (θ, I) be coordinates on Ξ_ε).

4.10 Discretization and Implementation

When implementing the previously-described methods on a computer, it is necessary to discretize all the functions used as well as the operations on them. We represent K, P, Λ, and other functions of θ as arrays of their values on a discrete grid of N evenly spaced θ values $\theta_i = 2\pi i/N$, $i = 0, \ldots, N-1$. Many operations on functions can be carried out element-wise on these arrays; such operations include

Fig. 1 Schematic of crossing gaps during ω continuation (consider the $\theta = 0$ and $\theta = 2\pi$ lines to be glued together to form a cylinder)

basic scalar arithmetic, matrix multiplication, and matrix inversion. For instance, given arrays of values $P(\theta_i)$ and $\xi(\theta_i)$, we can calculate a new array of N values $\Delta K(\theta_i) = P(\theta_i)\xi(\theta_i)$ (note that the ΔK array will actually contain $4N$ floating point numbers, since each $\Delta K(\theta_i) \in \mathbb{R}^4$).

Other operations must be carried out using Fourier coefficients. For instance, given an array of function values $a(\theta_i)$ for some $a : \mathbb{T} \to \mathbb{R}$, we can use

$$a(\theta_i) = \frac{1}{N}\sum_{k=0}^{N-1} \hat{a}(k)e^{jk\theta_i} \to a(\theta_i + \omega) = \frac{1}{N}\sum_{k=0}^{N-1} [\hat{a}(k)e^{jk\omega}]e^{jk\theta_i} \tag{72}$$

$$a(\theta_i) = \frac{1}{N}\sum_{k=0}^{N-1} \hat{a}(k)e^{jk\theta_i} \to Da(\theta_i) = \frac{1}{N}\sum_{k=0}^{N-1} [jk\hat{a}(k)]e^{jk\theta_i} \tag{73}$$

to translate or differentiate a. We use the fast Fourier transform (FFT) to get N Fourier coefficients $\hat{a}(k)$, multiply each $\hat{a}(k)$ by $e^{jk\omega}$ (translation) or jk (differentiation), and then take the inverse FFT to get an array of values $a(\theta_i + \omega)$ or $Da(\theta_i)$. Solving cohomological equations like (30) also requires working with Fourier coefficients as described in Section 4.5.

A few numerical problems were experienced when programming the quasi-Newton method, due to the implementation of continuous functions on a discrete computer. Let $\text{Translate}_\omega(a(\theta_i))$ represent the array of $a(\theta_i + \omega)$ values found by applying the algorithm of Eq. (72) to the array of $a(\theta_i)$ values. The first problem was that $\text{Translate}_\omega(F(\theta_i)G(\theta_i)) \neq \text{Translate}_\omega(F(\theta_i)) \times \text{Translate}_\omega(G(\theta_i))$; in other words, multiplying two arrays and then translating the result gave a different result than first translating the two arrays and then multiplying the results. Of course, when dealing with continuous functions, the order of multiplication and translation does not matter. Also, $F(\theta_i) \neq \text{Translate}_{-\omega}(\text{Translate}_{+\omega}(F(\theta_i)))$ when N is even and real-to-complex FFT is used (for real data).

These issues can prevent the convergence of our quasi-Newton method. It can be shown, however, that both inequalities are most pronounced when the high-

Fig. 2 Continuation of 5:6 Jupiter-Europa PERTBP resonant torus from $\varepsilon = 0$ to 0.0094

frequency Fourier coefficients of F or G are large in magnitude. It is not expected that the tori or bundles we compute should have significant high-frequency oscillations as a function of θ. Hence, a solution to these two problems we found was to run $K(\theta_i)$ and $P(\theta_i)$ through a lowpass filter when the method would start diverging, as well as between continuation steps. We also found that modifying P between continuation steps to make Λ constant, as described in Section 4.7, greatly mitigates these numerical issues as well.

4.11 Numerical Results in the PERTBP

We implemented and successfully applied the methods described in the previous several sections to the computation of invariant circles and their bundles for the Jupiter-Europa PERTBP stroboscopic map. The circles and bundles were found by first continuing Jupiter-Europa PCRTBP unstable resonant periodic orbits by eccentricity ε to $\varepsilon = 0.0094$ (the real value) for fixed ω, and then continuing the circles and bundles by ω while fixing $\varepsilon = 0.0094$.

Both 3:4 as well as 5:6 resonant tori were computed. Figure 2 shows the continuation by eccentricity of a 5:6 resonant periodic orbit from the PCRTBP to an invariant circle of the PERTBP stroboscopic map; for this, we used $N = 2048$ discretization θ_i values. The plot on the right zooms into the region near Europa; the leftmost curve there corresponds to $\varepsilon = 0.0094$, which is to be expected as Europa's periapsis moves leftwards as ε increases. Figure 3 shows the continuation of a 3:4 resonant torus in the physical $\varepsilon = 0.0094$ Jupiter-Europa PERTBP by ω. This yields a family of resonant tori in the system for $\omega \in [1.536217, 1.567314]$; N ranged from 1024 to 32768, with larger N required near the singularity at Europa.

After computing tori in the physical Jupiter-Europa PERTBP with $\varepsilon = 0.0094$, we also tested our quasi-Newton method to see if it would work for larger ε. Figure 4 shows selected tori from the continuation of a 3:4 resonant periodic orbit from the PCRTBP to an invariant circle of the PERTBP with Jupiter-Europa mass ratio μ, but $\varepsilon = 0.206$. This eccentricity is larger than that of the Sun-Mercury

Fig. 3 Continuation of $\varepsilon = 0.0094$ PERTBP 3:4 resonant tori by ω (Europa surface shown as red circle)

Fig. 4 Selected tori from 3:4 Jupiter-Europa PERTBP continuation from $\varepsilon = 0$ to 0.206

system, which has one of the most eccentric two-body orbits of any pair of large solar system bodies. We used $N = 1024$ and a continuation step size of $\Delta\varepsilon = 0.0005$ (the quasi-Newton method failed to converge for larger step sizes); every 20th torus is shown in the figure. As can be seen, our method was robust even for large values of the perturbation ε. On a 2017-era quad-core i7 laptop CPU, our Julia program took only about 230 seconds for the entire continuation to $\varepsilon = 0.206$, and less than 10 s for continuation to the physical value $\varepsilon = 0.0094$.

5 Parameterization Method for Stable and Unstable Manifolds

With the invariant circles and their stable and unstable bundles computed, we next turn our attention to accurate computation of torus stable and unstable manifolds. Many studies using manifolds, such as Olikara (2016), use linear approximations of invariant manifolds found by adding small vectors in the stable or unstable directions to the points of the torus, and then integrating backwards or forwards. However, we compute high order Fourier-Taylor polynomials which approximate the manifolds very accurately in some domain of validity. The algorithm used here bears many similarities with the method used in previous work (Kumar et al. 2021a) for computation of 1D manifolds of period-maps for periodic orbits in the PCRTBP. A different version of this algorithm was also used by Zhang and de la Llave (2018) in a lower-dimensional setting.

Since our F-invariant circles are 1D and have one stable and one unstable direction at each point, the circles' stable and unstable manifolds will be 2D and diffeomorphic to either an infinite cylinder or a Mobius strip. A cylinder can be continuously parameterized using an angle θ and a real number s; this actually is also possible for a Mobius strip, as long as the parameterization is non-injective and wraps around the strip twice as θ goes from 0 to 2π (the "double covering" trick we used in Section 4.8). In the framework of Section 4.1, we have $\mathcal{M} = \mathbb{T} \times \mathbb{R}$ and $f(\theta, s) = (\theta + \omega, \lambda s)$, where λ is the stable λ_s or unstable λ_u entry of Λ, depending on which manifold we are trying to compute. Without loss of generality, we assume that λ_s and λ_u are constant (see Section 4.7). With this, the equation to solve for the parameterization $W : \mathbb{T} \times \mathbb{R} \to \mathbb{R}^4$ of the stable or unstable manifold is

$$F(W(\theta, s)) - W(\theta + \omega, \lambda s) = 0, \quad (\theta, s) \in \mathbb{T} \times \mathbb{R} \tag{74}$$

5.1 Order-by-Order Method to find W

We express W as a Fourier-Taylor series of form

$$W(\theta, s) = K(\theta) + \sum_{k \geq 1} W_k(\theta) s^k \tag{75}$$

where $s = 0$ corresponds to the invariant circle $K(\theta)$ whose manifold we are trying to compute. The s^0 term of W is $K(\theta)$, and the linear term $W_1(\theta)$ is the stable $\mathbf{v}_s(\theta)$ or unstable $\mathbf{v}_u(\theta)$ bundle known from the third or fourth column of P. Hence we need to solve for the higher-order "coefficients" $W_k(\theta) : \mathbb{T} \to \mathbb{R}^4$, $k \geq 2$.

Denote $W_{<k}(\theta, s) = K(\theta) + \sum_{j=1}^{k-1} W_j(\theta) s^j$. Assume we have solved for all $W_j(\theta)$ for $j < k$, so that $F(W_{<k}(\theta, s)) - W_{<k}(\theta + \omega, \lambda s)$ has only s^k and higher order terms. Then, starting with $k = 2$, the recursive method to solve for $W_k(\theta)$ is:

1. Find $E_k(\theta) = [F(W_{<k}(\theta, s)) - W_{<k}(\theta + \omega, \lambda s)]_k$, where $[\cdot]_k$ denotes the s^k coefficient of the term inside brackets. We show how to do this in Section 5.2.
2. Find $W_k(\theta)$ such that $W_{<k}(\theta, s) + W_k(\theta) s^k$ cancels $E_k(\theta) s^k$ in Eq. (74), thus satisfying Eq. (74) up to order s^k. The equation to solve for $W_k(\theta)$ is

$$DF(K(\theta)) W_k(\theta) - \lambda^k W_k(\theta + \omega) = -E_k(\theta) \tag{76}$$

To solve this, let $W_{k,0} = 0$ and iterate the following sequence to convergence:

$$W_{k,i+1}(\theta) = \begin{cases} \lambda^k DF(K(\theta))^{-1} W_{k,i}(\theta + \omega) - DF(K(\theta))^{-1} E_k(\theta) & \text{if } |\lambda| < 1 \\ \lambda^{-k} DF(K(\theta - \omega)) W_{k,i}(\theta - \omega) + \lambda^{-k} E_k(\theta - \omega) & \text{if } |\lambda| > 1 \end{cases} \tag{77}$$

3. Set $W_{<k+1}(\theta, s) = W_{<k}(\theta, s) + W_k(\theta)s^k$ and return to step 1.

The recursion is stopped when we are satisfied with the degree k of W. We now prove that the equations and method described in Step 2 to find W_k are valid.

Claim If W_k solves Eq. (76), then for $j \leq k$ (using the $[\cdot]_k$ notation defined earlier),

$$\left[F(W_{<k}(\theta, s) + W_k(\theta)s^k) - \left(W_{<k}(\theta+\omega, \lambda s) + W_k(\theta+\omega)(\lambda s)^k\right)\right]_j = 0 \tag{78}$$

Proof Recall that $F(W_{<k}(\theta, s)) - W_{<k}(\theta+\omega, \lambda s) = E_k(\theta)s^k + O(s^{k+1})$. Expanding Eq. (78) in Taylor series and keeping only s^k and lower order terms gives

$$\begin{aligned}
&\Big[F(W_{<k}(\theta, s)) + DF(W_{<k}(\theta, s))W_k(\theta)s^k - \\
&\qquad\qquad \left(W_{<k}(\theta+\omega, \lambda s) + W_k(\theta+\omega)(\lambda s)^k\right)\Big]_j \\
&= [E_k(\theta)s^k + DF(W_{<k}(\theta, s))W_k(\theta)s^k - \lambda^k W_k(\theta+\omega)s^k]_j \\
&= \begin{cases} 0 & \text{if } j < k, \\ E_k(\theta) + DF(K(\theta))W_k(\theta) - \lambda^k W_k(\theta+\omega) = 0 & \text{if } j = k \end{cases}
\end{aligned} \tag{79}$$

where the $j = k$ case of the last line follows from the preceding line by dividing s^k out from the quantity inside $[.]_j$, and then taking $s \to 0$. □

Claim The sequence $\{W_{k,i}\}_{i\in\mathbb{N}}$ defined by $W_{k,0} = 0$ and Eq. (77) converges to W_k.

$$W_{k,i+1}(\theta) = \begin{cases} \lambda^k DF(K(\theta))^{-1} W_{k,i}(\theta+\omega) - DF(K(\theta))^{-1} E_k(\theta) & \text{if } |\lambda| < 1 \\ \lambda^{-k} DF(K(\theta-\omega)) W_{k,i}(\theta-\omega) + \lambda^{-k} E_k(\theta-\omega) & \text{if } |\lambda| > 1 \end{cases} \tag{80}$$

Proof Let P, Λ be the bundle and Floquet matrices for $K(\theta)$. We assume that Λ is constant (as the procedure from Section 4.7 gives). Then, it is easy to show that

$$W_{k,i}(\theta) = \begin{cases} -P(\theta)\sum_{j=0}^{i-1} \lambda^{kj} \Lambda^{-j-1} [P^{-1}(\theta+(j+1)\omega)E_k(\theta+j\omega)] & \text{if } |\lambda| < 1 \\ P(\theta)\sum_{j=0}^{i-1} \lambda^{-k(j+1)} \Lambda^{j} [P^{-1}(\theta-j\omega)E_k(\theta-(j+1)\omega)] & \text{if } |\lambda| > 1 \end{cases} \tag{81}$$

solves Eq. (77) with $W_{k,0} = 0$; simply substitute Eq. (81) for $W_{k,i}$ in Eq. (77) and use $DF(K(\theta-\omega))P(\theta-\omega) = P(\theta)\Lambda$ and $DF(K(\theta))^{-1} = P(\theta)\Lambda^{-1}P^{-1}(\theta+\omega)$ to simplify the RHS of the resulting equation.

Now, we will show that $W_k(\theta) = \lim_{i\to\infty} W_{k,i}(\theta)$. First of all, note that

$$\lambda_s^j \Lambda^{-j} = \begin{bmatrix} \lambda_s^j & -j\lambda_s^j T & 0 & 0 \\ 0 & \lambda_s^j & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \lambda_s^j \lambda_u^{-j} \end{bmatrix} \qquad \lambda_u^{-j} \Lambda^{j} = \begin{bmatrix} \lambda_u^{-j} & j\lambda_u^{-j} T & 0 & 0 \\ 0 & \lambda_u^{-j} & 0 & 0 \\ 0 & 0 & \lambda_s^j \lambda_u^{-j} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{82}$$

for all $j \in \mathbb{N}$, where Λ is of the form given in Eq. (12) and has constant T, λ_s, and λ_u as assumed earlier. Since $|\lambda_s| < 1$ and $|\lambda_u| > 1$, $\lambda_s^j \Lambda^{-j}$ and $\lambda_u^{-j} \Lambda^j$ are hence bounded for all $j \in \mathbb{N}$. Now, define $\Gamma_s(\theta) = \Lambda^{-1}P^{-1}(\theta+\omega)E_k(\theta)$ and $\Gamma_u(\theta) = \lambda^{-k}P^{-1}(\theta)E_k(\theta-\omega)$; also, recall that $|\lambda| < 1$ means $\lambda = \lambda_s$ and $|\lambda| > 1$ means $\lambda = \lambda_u$. We can use all this to rewrite Eq. (81) as

$$W_{k,i}(\theta) = \begin{cases} -P(\theta)\sum_{j=0}^{i-1} \lambda_s^{(k-1)j} [\lambda_s^j \Lambda^{-j} \Gamma_s(\theta+j\omega)] & \text{if } |\lambda| < 1 \\ P(\theta)\sum_{j=0}^{i-1} \lambda_u^{-(k-1)j} [\lambda_u^{-j} \Lambda^{j} \Gamma_u(\theta-j\omega)] & \text{if } |\lambda| > 1 \end{cases} \tag{83}$$

In both $|\lambda| < 1$ and $|\lambda| > 1$ cases of Eq. (83), the quantities in square brackets are bounded for all $\theta \in \mathbb{T}$ and $j \in \mathbb{N}$. As $k \geq 2$, $\lambda_s^{k-1} < 1$ and $\lambda_u^{-(k-1)} < 1$; hence, if $i \to \infty$, the sum in Eq. (83) is absolutely uniformly convergent. Hence $L(\theta) = \lim_{i \to \infty} W_{k,i}(\theta)$ exists. Letting $i \to \infty$ on both sides of Eq. (77) gives

$$L(\theta) = \begin{cases} \lambda^k DF(K(\theta))^{-1} L(\theta + \omega) - DF(K(\theta))^{-1} E_k(\theta) & \text{if } |\lambda| < 1 \\ \lambda^{-k} DF(K(\theta - \omega)) L(\theta - \omega) + \lambda^{-k} E_k(\theta - \omega) & \text{if } |\lambda| > 1 \end{cases} \tag{84}$$

which for both $|\lambda| < 1$ and $|\lambda| > 1$ is equivalent to Eq. (76) with $W_k = L$. $\square$

Remark 6 Given P and Λ satisfying Eq. (11), substituting $W_k = PV_k$ into Eq. (76) and rearranging gives $\Lambda V_k(\theta) - \lambda^k V_k(\theta + \omega) = -P(\theta + \omega)^{-1} E_k(\theta)$, which can be solved for V_k component by component using the Fourier methods from Section 4.5.2. We used the iteration method of Eq. (77) instead, to avoid any possible multiplication-translation numerical discretization issues (see Section 4.10).

5.2 Computing $E_k(\theta)$: Automatic Differentiation and Jet Transport

In step 1 of the order-by-order method to find W, we compute the s^k coefficient

$$E_k(\theta) = [F(W_{<k}(\theta, s)) - W_{<k}(\theta + \omega, \lambda s)]_k \tag{85}$$

$W_{<k}(\theta, s)$ is a Fourier-Taylor series with terms up to order s^{k-1}, and λ is a constant, so the s^k term of $W_{<k}(\theta + \omega, \lambda s)$ is 0. However, F is a nonlinear stroboscopic map defined by integrating points for a fixed time $2\pi/\Omega_p$ by the equations of motion (3) and (4). Hence, computing $F(W_{<k}(\theta, s))$ as a Fourier-Taylor series is not a trivial matter. For this, the tools of automatic differentiation (Haro et al. 2016) and jet transport (Pérez-Palau et al. 2015) are useful. Note that some researchers (Rasotto et al. 2016; Berz and Makino 1998) use the term differential algebra to refer to what we call automatic differentiation. The exposition in this and the next few sections closely mirrors that of our previous work (Kumar et al. 2021a).

Automatic differentiation is a technique which allows for rapid recursive evaluation of operations on Taylor series. For instance, given two series $f(s)$ and $g(s)$, $s \in \mathbb{R}$, suppose we wish to compute the Taylor series for $d(s) = f(s)/g(s)$. We know that $d(s) = f(s)/g(s) \iff f(s) = d(s)g(s)$; hence, using subscript j to denote the coefficient of s^j in the series, we find that

$$f_i(s) = \sum_{j=0}^{i} d_j(s) g_{i-j}(s) = \left(\sum_{j=0}^{i-1} d_j(s) g_{i-j}(s) \right) + d_i(s) g_0(s) \tag{86}$$

$$\therefore d_i(s) = \frac{1}{g_0} \left(f_i(s) - \sum_{j=0}^{i-1} d_j(s) g_{i-j}(s) \right) \tag{87}$$

We know that $d_0 = f_0/g_0$; using Eq. (87) with the known coefficients of f and g, we can recursively find $d_i(s)$, $k \geq 1$. Similar recursive formulas exist for $f(s)^\alpha$, $\alpha \in \mathbb{R}$, as well as many other functions and operations; these can be found in Haro et al. (2016). The key property of all automatic differentiation formulas is that the s^k coefficient of the output depends only on the s^k and lower order coefficients of the operands. Hence, we can use truncated Taylor series with these algorithms when implementing them in computer programs.

Recall from Section 4.10 that on the computer, we represent all functions of θ, including the $W_j(\theta)$, as arrays of function values on an evenly spaced grid of θ values $\theta_i = 2\pi i/N$, $i = 0, \ldots, N-1$. Note that for fixed θ_i, $W_{<k}(\theta_i, s)$ is a Taylor series (not Fourier-Taylor) with coefficients $W_j(\theta_i) \in \mathbb{R}^4$. The utility of automatic differentiation is that it allows us to substitute Taylor series such as $W_{<k}(\theta_i, s)$ for (x, y, p_x, p_y) in the equations of motion (3) to get series in s for $(\dot{x}, \dot{y}, \dot{p}_x, \dot{p}_y)$. In terms of computer programming, this means that after overloading the required operators (usually arithmetic and power) to accept Taylor series arguments, we can use numerical integration routines with the series as well.

To be more clear, consider $V(s,t) = \sum_{j=0}^{\infty} V_j(t) s^j : \mathbb{R}^2 \to \mathbb{R}^4$ as a Taylor series-valued function of time, with time-varying coefficients $V_j(t)$. Denote the x, y, p_x, and p_y components of $V(s,t)$ as $V_x(s,t)$, $V_y(s,t)$, $V_{p_x}(s,t)$, and $V_{p_y}(s,t)$; similarly write $V_{j,x}(t)$, $V_{j,y}(t)$, $V_{j,p_x}(t)$, and $V_{j,p_y}(t)$ for the components of $V_j(t)$. Substituting V in the equations of motion, we get the system of differential equations

$$\frac{d}{dt} V_x(s,t) = \sum_{j=0}^{\infty} \dot{V}_{j,x}(t) s^j = \frac{\partial H_\varepsilon}{\partial p_x}\Big(V_x(s,t), V_y(s,t), V_{p_x}(s,t), V_{p_y}(s,t), \theta_p\Big) \tag{88}$$

$$\frac{d}{dt} V_y(s,t) = \sum_{j=0}^{\infty} \dot{V}_{j,y}(t) s^j = \frac{\partial H_\varepsilon}{\partial p_y}\Big(V_x(s,t), V_y(s,t), V_{p_x}(s,t), V_{p_y}(s,t), \theta_p\Big) \tag{89}$$

$$\frac{d}{dt} V_{p_x}(s,t) = \sum_{j=0}^{\infty} \dot{V}_{j,p_x}(t) s^j = -\frac{\partial H_\varepsilon}{\partial x}\Big(V_x(s,t), V_y(s,t), V_{p_x}(s,t), V_{p_y}(s,t), \theta_p\Big) \tag{90}$$

$$\frac{d}{dt} V_{p_y}(s,t) = \sum_{j=0}^{\infty} \dot{V}_{j,p_y}(t) s^j = -\frac{\partial H_\varepsilon}{\partial y}\Big(V_x(s,t), V_y(s,t), V_{p_x}(s,t), V_{p_y}(s,t), \theta_p\Big) \tag{91}$$

$$\dot{\theta}_p = \Omega_p \tag{92}$$

H_ε and its partials are algebraic functions that are suitable for use with automatic differentiation techniques; see, for instance, the PERTBP Hamiltonian Eq. (5). Hence, if the $V_{j,x}(t)$, $V_{j,y}(t)$, $V_{j,p_x}(t)$, $V_{j,p_y}(t)$, and θ_p are known for $j \in \mathbb{N}$ and some $t \in \mathbb{R}$, the RHS of each of Eq. (88)-(91) can be simplified to a series in s using automatic differentiation. Then, for each of Eq. (88)-(91) and $j \in \mathbb{N}$, the s^j coefficient $\dot{V}_{j,x}(t)$, $\dot{V}_{j,y}(t)$, $\dot{V}_{j,p_x}(t)$, or $\dot{V}_{j,p_y}(t)$ from the LHS must be equal to the s^j coefficient of the RHS. In other words, $\dot{V}_{j,x}(t)$, $\dot{V}_{j,y}(t)$, $\dot{V}_{j,p_x}(t)$, and $\dot{V}_{j,p_y}(t)$, $j \in \mathbb{N}$, are functions of θ_p, $V_{j,x}(t)$, $V_{j,y}(t)$, $V_{j,p_x}(t)$, and $V_{j,p_y}(t)$, $j \in \mathbb{N}$. This can be interpreted as a system of differential equations for the time-varying Taylor coefficients of $V(s,t)$. Solving this equation with initial condition $V(s,0) = W_{<k}(\theta_i, s)$ and initial θ_p equal to the value fixed in Section 3.1, we have that $V(s, 2\pi/\Omega_p) = F(W_{<k}(\theta_i, s))$, which is the series we need.

Hence, by treating the coefficients of $W_{<k}(\theta_i, s)$ as initial state variables to be integrated from 0 to $2\pi/\Omega_p$, we can numerically integrate $W_{<k}(\theta_i, s)$ coefficient by coefficient to find the Taylor coefficients of $F(W_{<k}(\theta_i, s))$. We do this for each $i = 0, \ldots, N-1$, which is enough to represent the Fourier-Taylor coefficients of $F(W_{<k}(\theta, s))$ on the computer; the s^k coefficient of this gives us $E_k(\theta)$. This method of integrating a polynomial curve is known as jet transport; for more details, see

Pérez-Palau et al. (2015). We can use truncated Taylor series with jet transport, since the automatic differentiation formulas used for the evaluation of time derivatives are valid for truncated series. Note that if we have an n-dimensional state ($n = 4$ in our case) and a degree-d truncated series, then the integration required is $n(d+1)$ dimensional.

5.3 Notes About Numerical Computation of Manifolds

The parameterization method, automatic differentiation, and jet transport described in the preceding sections were implemented in a C program for the computation of stable and unstable manifolds. For numerical integration, including jet transport, we used the Runge-Kutta Prince-Dormand (8,9) integrator from the GSL library (Galassi et al. 2009); integrations were parallelized using OpenMP with one thread for each θ_i value. We tested our tools by computing manifolds of some of the 3:4 and 5:6 Jupiter-Europa PERTBP tori shown in Fig. 2 and 3, with N ranging from 1024 to 2048. On a quad-core Intel i7 laptop CPU, the program took less than 10 seconds for the computation of s^5-order parameterizations.

Note that in each step of order k, when $F(W_{<k}(\theta_i, s)) - W_{<k}(\theta_i + \omega, \lambda s)$ is computed in order to find $E_k(\theta_i)$, the s^j coefficients for $j < k$ should be zero (to compute the $W_{<k}(\theta_i + \omega, \lambda s)$ coefficients, use the translation algorithm from Section 4.10 on the arrays of $W_j(\theta_i)$ values, and then multiply $W_j(\theta_i + \omega)$ by λ^j). This behavior was indeed observed when running the program, serving as a check on the accuracy of the computation. The final s^d-degree truncated series $W_{\leq d}(\theta, s) = K(\theta) + \sum_{j=1}^{d} W_j(\theta) s^j$ satisfies $F(W_{\leq d}(\theta_i, s)) - W_{\leq d}(\theta_i + \omega, \lambda s) = 0$ up to terms of order s^d, for each $i = 0, \ldots, N-1$.

To optimize computational time and storage requirements, at the $W_k(\theta)$ step, we truncate all series at s^k for the automatic differentiation and jet transport steps. Also, note that if $W(\theta, s)$ solves Eq. (74), then so does $W(\theta, \alpha s)$ where α is an arbitrary constant. Hence, if the jet transport integration is struggling to converge due to fast-growing coefficients $W_j(\theta)$ of $W(\theta, s)$, it helps to scale $W(\theta, s)$ to $W(\theta, \alpha s)$ by multiplying the stable or unstable bundle $W_1(\theta)$ by $\alpha < 1$ and then restarting the parameterization method algorithm.

Finally, one last remark is that in certain systems, such as the PERTBP with $\theta_p = 0$ at $t = 0$, the equations of motion have the same time-reversal symmetry as the PCRTBP. In this case, the unstable manifold $W^u(\theta, s)$ can be found from the stable manifold $W^s(\theta, s)$ simply by setting $W^u(\theta, s) = W^s(2\pi - \theta, s)$ and then multiplying the y and p_x components of $W^u(\theta, s)$ by -1. This enables us to save half of the computation time that computing both W^s and W^u would have taken.

5.4 Fundamental Domains of Parameterizations

Though the d degree Fourier-Taylor parameterizations $W_{\leq d}(\theta, s)$ of the manifolds of $K(\theta)$ will be more accurate than linear approximation by the stable or unstable direction vector at each point $K(\theta)$, they are still inexact and subject to series truncation error. In addition, even if the exact infinite series $W(\theta, s)$ satisfying Eq. (74) could be computed, it still would only be valid within some radius of convergence for s. Hence, one must determine for which values of $s \in \mathbb{R}$ the parameterization $W_{\leq d}(\theta, s)$ is an accurate representation of the invariant manifold.

To do this, we first fix an error tolerance, such as say $E_{tol} = 10^{-5}$ or 10^{-6}. We then seek to find what is referred to as the fundamental domain of $W_{\leq d}(\theta, s)$. The fundamental domain is defined as the largest set $\mathbb{T} \times (-D, D)$ such that for all $(\theta, s) \in \mathbb{T} \times (-D, D)$, the error in invariance Eq. (74) is less than E_{tol}. In other words, we want the largest $D \in \mathbb{R}^+$ such that for all s satisfying $|s| < D$,

$$\max_{\theta \in \mathbb{T}} \left\| F(W_{\leq d}(\theta, s)) - W_{\leq d}(\theta + \omega, \lambda s) \right\| < E_{tol} \tag{93}$$

In practice, since we know $K(\theta)$ and $W_j(\theta)$, $j = 1, \ldots, d$, at the values θ_i, $i = 0, \ldots, N-1$, we search for the largest $D \in \mathbb{R}^+$ such that for all s with $|s| < D$,

$$\max_{i=0,\ldots,N-1} \left\| F(W_{\leq d}(\theta_i, s)) - W_{\leq d}(\theta_i + \omega, \lambda s) \right\| < E_{tol} \tag{94}$$

The simplest way of finding D is to first use bisection to find the largest D_i such that $\left\| F(W_{\leq d}(\theta_i, s)) - W_{\leq d}(\theta_i + \omega, \lambda s) \right\| < E_{tol}$ for all $s \in (-D_i, D_i)$. After doing this for $i = 0, \ldots, N-1$, D will be the minimum of all the D_i.

By computing the fundamental domains of validity for 5 different 3:4 and 5:6 PERTBP resonant torus manifold parameterizations, we observed a 50-200 times increase in the domains for $d = 5$ compared to $d = 1$. For linear parameterizations ($d = 1$), the domain size D of all test cases was on the order of 10^{-4} at best, generally 10^{-5}. However, for the degree-5 polynomial parameterizations $W_{d \leq 5}(\theta, s)$, D was on the order of 10^{-3} or 0.01. Higher degree parameterizations may improve even further. Note that a larger fundamental domain means that less numerical integration is required for manifold globalization, reducing the computation time.

6 Globalization, Regularization, and Visualization

At this point, we have accurate local representations of stable and unstable manifolds of our stroboscopic map invariant circles. Given a manifold's Fourier-Taylor parameterization $W_P(\theta, s)$ and its fundamental domain $\mathcal{D} = \mathbb{T} \times (-D, D)$, the image $W_P(\mathcal{D})$ gives us a piece of the manifold in the map phase space $\mathbb{R}^4$. However, this subset of the manifold will be close to its base invariant circle $K(\theta)$; generally, it is motions on the manifold further away from the torus that are of interest for applications. Hence, we need to extend our Fourier-Taylor parameterization $W_P : \mathcal{D} \to \mathbb{R}^4$ to a function $W : \mathbb{T} \times \mathbb{R} \to \mathbb{R}^4$ parameterizing the entire manifold, with $W = W_P$ on $\mathcal{D}$. This is referred to as globalization.

Recall from Eq. (74) that W must satisfy $F(W(\theta, s)) = W(\theta + \omega, \lambda s)$. Applying this repeatedly, we have that $F^k(W(\theta, s)) = W(\theta + k\omega, \lambda^k s)$, where the superscript $k \in \mathbb{Z}^+$ refers to function composition. We can rewrite this as

$$W(\theta, s) = F^k(W(\theta - k\omega, \lambda^{-k} s)) \tag{95}$$

$$W(\theta, s) = F^{-k}(W(\theta + k\omega, \lambda^k s)) \tag{96}$$

Eq. (95) and (96) allow us to define $W(\theta, s)$ for all $(\theta, s) \in \mathbb{T} \times \mathbb{R}$. If W is an unstable manifold and hence $|\lambda| > 1$, choose $k \geq 0$ such that $|\lambda^{-k} s| < D$ and use W_P to evaluate the RHS of Eq. (95). Similarly, if W is a stable manifold with $|\lambda| < 1$, then take $k \geq 0$ such that $|\lambda^k s| < D$ and evaluate Eq. (96). The mapping F^k (or F^{-k}) is just a time $2\pi k/\Omega_p$ (or $-2\pi k/\Omega_p$) numerical integration. Also, $W(\theta, s)$ thus defined satisfies $F(W(\theta, s)) = W(\theta + \omega, \lambda s)$ for all $(\theta, s) \in \mathbb{T} \times \mathbb{R}$, so the image $W(\mathbb{T} \times \mathbb{R})$ is F-invariant. Hence, Eq. (95) and (96) give us a global representation of the entire unstable or stable manifold.

6.1 Mesh Representations of Globalized Manifolds

For visualization, we often want to calculate a mesh of many points on the manifold, rather than just a few $W(\theta, s)$ values. To do this, we first take an evenly-spaced grid of L s-values $\{s_j\}$ from $-D$ to D, in addition to our grid of N θ values θ_i, and then directly evaluate the Fourier-Taylor parameterization to compute $W(\theta_i, s_j)$ for each $i = 0, \dots, N-1$, $j = 1, \dots, L$. Next, we repeatedly apply F or F^{-1} to the $W(\theta_i, s_j)$ to get the points $W(\theta_i + k\omega, \lambda^k s_j) = F^k(W(\theta_i, s_j))$ if $|\lambda| > 1$ or $W(\theta_i - k\omega, \lambda^{-k} s_j) = F^{-k}(W(\theta_i, s_j))$ if $|\lambda| < 1$, for $k = 0, 1, 2, \dots$ up to some $k_{max} \in \mathbb{Z}^+$. The numerical integrations required in this step may require use of regularized equations of motion, which we will discuss in Section 6.2. Finally, we use the translation algorithm given in Eq. (72) to find the points $W(\theta_i, \lambda^k s_j)$ if $|\lambda| > 1$ or $W(\theta_i, \lambda^{-k} s_j)$ if $|\lambda| < 1$; we need all points to be at the same set of N θ_i values when trying to create a manifold mesh that can be plotted.

By following this procedure, we get a discretized, plottable representation of the manifold subset $\{W(\theta, s) : (\theta, s) \in \mathbb{T} \times [-M, M]\}$, where $M = \lambda^{k_{max}} D$ if $|\lambda| > 1$ and $M = \lambda^{-k_{max}} D$ if $|\lambda| < 1$. Note that the numerical integrations can be parallelized across θ_i values, which we took advantage of. A 3D projection of an example globalized stable manifold mesh (denoted W^s) of a 3:4 Jupiter-Europa PERTBP invariant circle is given in Figure 5, with $N = 1024$, $L = 101$, $k_{max} = 6$.

6.2 The Need for Regularization: An Extension of Levi-Civita to the PERTBP

In the equations of motion for the PERTBP and other periodically-perturbed PCRTBP models, the positions of the two large masses m_1 and m_2 correspond to singularities. However, when numerically integrating points forwards or backwards during the manifold mesh computation described in Section 6.1, it is possible for some points' trajectories to pass extremely close to the singularity at m_2. Moreover, this can indicate that the manifold being computed actually passes through the m_2 singularity. Such behavior was observed, for example, during computation of manifold meshes for 5:6 Jupiter-Europa PERTBP tori. These close approaches to m_2 can result in numerical issues, including lack of integrator convergence.

In the PCRTBP, the Levi-Civita regularization is very commonly used to compute trajectories which pass near or through a singularity; see Celletti (2010) for full details. First, a canonical coordinate transformation is applied to the PCRTBP Hamiltonian H_0 from Eq. (2). This is followed by the addition of a pair of action-angle variables to the transformed Hamiltonian; the new action's value is set to $-H_0$, which has a constant value along the trajectory. This finally allows a time-rescaling to be used which cancels the singularity. This method, however, relies on the fact that H_0 is constant along PCRTBP trajectories. For our periodically-perturbed models, this is not the case. Hence, some modification is required.

Fig. 5 (x, y, p_x) projection of Jupiter-Europa PERTBP 3:4 W^s for $\omega = 1.559620297$

For the PERTBP, the singularity corresponding to m_2 is the time-varying point $(x, y) = ((1-\mu)(1-\varepsilon \cos E(t)), 0)$. We now present the derivation of the modified Levi-Civita regularization of m_2 for the PERTBP; we expect very similar methods to apply for other periodically-perturbed PCRTBP models as well. Readers primarily interested in using the final regularized equations for numerical integration should skip to Section (6.2.1). The following is heavily inspired by Celletti (2010).

First, take the PERTBP Hamiltonian H_ε from Eq. (5) and add a momentum variable p_t conjugated to t. The Hamiltonian and equations of motion become

$$\bar{H}_\varepsilon(p_x, p_y, p_t, x, y, t) = p_t + \frac{p_x^2 + p_y^2}{2} + n(t)(p_x y - p_y x) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2} \tag{97}$$

$$\dot{x} = \frac{\partial \bar{H}_\varepsilon}{\partial p_x} \quad \dot{y} = \frac{\partial \bar{H}_\varepsilon}{\partial p_y} \quad \dot{t} = \frac{\partial \bar{H}_\varepsilon}{\partial p_t} \qquad \dot{p}_x = -\frac{\partial \bar{H}_\varepsilon}{\partial x} \quad \dot{p}_y = -\frac{\partial \bar{H}_\varepsilon}{\partial y} \quad \dot{p}_t = -\frac{\partial \bar{H}_\varepsilon}{\partial t} \tag{98}$$

where $r_1 = \sqrt{\big(x + \mu(1+\chi(t))\big)^2 + y^2}$, $r_2 = \sqrt{\big(x - (1-\mu)(1+\chi(t))\big)^2 + y^2}$, and $\chi(t) = -\varepsilon \cos E(t)$. Note that adding p_t does not change the values of $\dot{x}$, $\dot{y}$, $\dot{p}_x$, $\dot{p}_y$, and $\dot{t} = \partial \bar{H}_\varepsilon / \partial p_t = 1$ as compared to using Eq. (5). However, unlike H_ε, the new Hamiltonian $\bar{H}_\varepsilon$ does remain constant along trajectories in (p_x, p_y, p_t, x, y, t) space. Also, given an initial condition (x, y, p_x, p_y, t) to be propagated, the initial value of p_t should be set so that $\bar{H}_\varepsilon = 0$; this will be important later on.

Now, we do a canonical coordinate transformation. Define a generating function

$$W(p_x, p_y, p_t, X, Y, T) = p_x \Big(X^2 - Y^2 + (1-\mu)(1+\chi(T))\Big) + p_2(2XY) + p_t T \tag{99}$$

which is a function of the old momenta and new configuration space coordinates. Then, this defines a transformation between the old (p_x, p_y, p_t, x, y, t) variables and new (P_X, P_Y, P_T, X, Y, T) variables through the relations (Thirring 1992)

$$\begin{aligned} x &= \frac{\partial W}{\partial p_x} = X^2 - Y^2 + (1-\mu)(1+\chi(T)) & y &= \frac{\partial W}{\partial p_y} = 2XY \\ P_X &= \frac{\partial W}{\partial X} = 2p_x X + 2p_y Y & P_Y &= \frac{\partial W}{\partial Y} = -2p_x Y + 2p_y X \\ t &= \frac{\partial W}{\partial p_t} = T & P_T &= \frac{\partial W}{\partial T} = (1-\mu)p_x \frac{d\chi}{dt}(T) + p_t \end{aligned} \tag{100}$$

Eq. (100) gives us x, y, and t in terms of the new variables. We can also solve for p_x and p_y to get $p_x = \frac{2}{R}(P_X X - P_Y Y)$ and $p_y = \frac{2}{R}(P_X Y + P_Y X)$, where $R = 4(X^2 + Y^2)$. This then gives us $p_t = P_T - \frac{2}{R}(1-\mu)(P_X X - P_Y Y)\frac{d\chi}{dt}(T)$. Note that in the new variables, $r_2 = \sqrt{(X^2 - Y^2)^2 + (2XY)^2} = R/4$.

Substituting the previous expressions for (p_x, p_y, p_t, x, y, t) into Eq. (97) gives

$$\begin{aligned} &\hat{H}_\varepsilon(P_X, P_Y, P_T, X, Y, T) = \\ &\qquad P_T - \frac{2}{R}(1-\mu)(P_X X - P_Y Y)\frac{d\chi}{dt}(T) + \frac{P_X^2 + P_Y^2}{2R} \\ &\qquad + 2n(T)\left[\frac{1}{4}(P_X X - P_Y Y) - \frac{(1-\mu)}{R}(1+\chi(T))(P_X Y + P_Y X)\right] \\ &\qquad - \frac{1-\mu}{\sqrt{(X^2+Y^2)^2 + (1+\chi(T))^2 + 2(X^2-Y^2)(1+\chi(T))}} - \frac{4\mu}{R} \end{aligned} \tag{101}$$

The m_2 singularity is now at $(X, Y) = (0, 0)$, where $R = 4r_2 = 0$. Since this was a canonical transformation, the equations of motion in the new coordinates will be

$$\dot{X} = \frac{\partial \hat{H}_\varepsilon}{\partial P_X} \quad \dot{Y} = \frac{\partial \hat{H}_\varepsilon}{\partial P_Y} \quad \dot{T} = \frac{\partial \hat{H}_\varepsilon}{\partial P_T} \quad \dot{P}_X = -\frac{\partial \hat{H}_\varepsilon}{\partial X} \quad \dot{P}_Y = -\frac{\partial \hat{H}_\varepsilon}{\partial Y} \quad \dot{P}_T = -\frac{\partial \hat{H}_\varepsilon}{\partial T} \tag{102}$$

To regularize the singularity at $R = 0$, we want to be able to use $R\hat{H}_\varepsilon$ instead of $\hat{H}_\varepsilon$. For this, define a rescaled time s such that $dt = R\,ds$. Then, we have that $\frac{d}{ds} = \frac{d}{dt}\frac{dt}{ds} = R\frac{d}{dt}$. Thus, letting prime ($'$) denote d/ds,

$$\begin{aligned} X' &= R\frac{\partial \hat{H}_\varepsilon}{\partial P_X} \quad & Y' &= R\frac{\partial \hat{H}_\varepsilon}{\partial P_Y} \quad & T' &= R\frac{\partial \hat{H}_\varepsilon}{\partial P_T} \\ P_X' &= -R\frac{\partial \hat{H}_\varepsilon}{\partial X} \quad & P_Y' &= -R\frac{\partial \hat{H}_\varepsilon}{\partial Y} \quad & P_T' &= -R\frac{\partial \hat{H}_\varepsilon}{\partial T} \end{aligned} \tag{103}$$

Since R is a function of only X and Y, it is immediate that $X' = \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_X}$, $Y' = \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_Y}$, $T' = \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_T}$, and $P_T' = -\frac{\partial[R\hat{H}_\varepsilon]}{\partial T}$. Furthermore, since p_t was chosen earlier to ensure $\bar{H}_\varepsilon = 0$, we also will have $\hat{H}_\varepsilon = 0$ along the trajectory in (P_X, P_Y, P_T, X, Y, T) space. Hence, we find that $\frac{\partial[R\hat{H}_\varepsilon]}{\partial X} = R\frac{\partial \hat{H}_\varepsilon}{\partial X} + \hat{H}_\varepsilon\frac{\partial R}{\partial X} = R\frac{\partial \hat{H}_\varepsilon}{\partial X}$. This yields $P_X' = -\frac{\partial[R\hat{H}_\varepsilon]}{\partial X}$; we similarly find $P_Y' = -\frac{\partial[R\hat{H}_\varepsilon]}{\partial Y}$. As $R\hat{H}_\varepsilon$ has no singularity at $R = 0$, we thus obtain the m_2-regularized time-s equations of motion

$$\begin{aligned} X' &= \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_X} \quad & Y' &= \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_Y} \quad & T' &= \frac{\partial[R\hat{H}_\varepsilon]}{\partial P_T} \\ P_X' &= -\frac{\partial[R\hat{H}_\varepsilon]}{\partial X} \quad & P_Y' &= -\frac{\partial[R\hat{H}_\varepsilon]}{\partial Y} \quad & P_T' &= -\frac{\partial[R\hat{H}_\varepsilon]}{\partial T} \end{aligned} \tag{104}$$

6.2.1 Usage of Regularized PERTBP Equations of Motion

Let (x^i, y^i, p_x^i, p_y^i) be an initial state we wish to integrate from $t = t_i$ to t_f in the PERTBP. Recall H_ε from Eq. (5), and $\bar{H}_\varepsilon$ from Eq. (97), with $\chi(t) = -\varepsilon \cos E(t)$. To use the m_2-regularized equations of motion for this integration, we:

1. Set $p_t^i = -H_\varepsilon(p_x^i, p_y^i, x^i, y^i, t_i)$, so that $\bar{H}_\varepsilon(p_x^i, p_y^i, p_t^i, x^i, y^i, t_i) = 0$.
2. Compute initial $(P_X^i, P_Y^i, P_T^i, X^i, Y^i, T^i)$ using the equations (where $j = \sqrt{-1}$)

$$\begin{aligned} &X + jY = \big(x - (1-\mu)(1+\chi(t)) + jy\big)^{1/2} \\ P_X =& 2p_x X + 2p_y Y \qquad P_Y = -2p_x Y + 2p_y X \\ &T = t \qquad P_T = (1-\mu) p_x \frac{d\chi}{dt}(t_1) + p_t \end{aligned} \tag{105}$$

   The sign chosen during the complex square root for $X + jY$ does not matter.
3. Integrate the initial condition $(P_X^i, P_Y^i, P_T^i, X^i, Y^i, T^i)$ using Eq. (104), where $R = 4(X^2 + Y^2)$ and $\hat{H}_\varepsilon$ is given by Eq. (101). Only stop the integration when $T = t_f$; do not stop before this occurs, even if the integration time reaches t_2.
4. Transform the resulting final state back to (p_x, p_y, p_t, x, y, t) coordinates using

$$\begin{aligned} x &= X^2 - Y^2 + (1-\mu)(1+\chi(T)) \qquad y = 2XY \\ p_x &= \frac{2}{R}(P_X X - P_Y Y) \qquad p_y = \frac{2}{R}(P_X Y + P_Y X) \\ t &= T = t_2 \qquad p_t = P_T - \frac{2}{R}(1-\mu)(P_X X - P_Y Y)\frac{d\chi}{dt}(T) \end{aligned} \tag{106}$$

The first line of Eq. (105) should be interpreted as two real equations corresponding to setting real and imaginary parts of both sides equal. It follows from the first line of Eq. (100) combined with the relation $(X + jY)^2 = X^2 - Y^2 + j(2XY)$. Also, for step 3 above, the requirement to stop integration when $T = t_f$ can be implemented using the "events" functionality of MATLAB's ODE solvers, or the callback features in Julia's DifferentialEquations.jl library.

The partial derivatives of $R\hat{H}_\varepsilon$ appearing in the equations of motion Eq. (104) are straightforward to compute but lengthy, so we do not write them here. Throughout the steps listed above, as well as for computing the partial derivatives, we need the quantities $\frac{d\chi}{dt}$, $\frac{d^2\chi}{dt^2}$, and $\frac{dn}{dt}$. These are given by the equations

$$\frac{d\chi}{dt} = \frac{\varepsilon \sin E}{1 - \varepsilon \cos E} \qquad \frac{d^2\chi}{dt^2} = \frac{\varepsilon \cos E - \varepsilon^2}{(1 - \varepsilon \cos E)^3} \qquad \frac{dn}{dt} = \frac{-2\varepsilon\sqrt{1-\varepsilon^2}}{(1 - \varepsilon \cos E)^4} \sin E$$

which can be derived from $\chi(t) = -\varepsilon \cos E(t)$, $n(t) = \frac{\sqrt{1-\varepsilon^2}}{(1-\varepsilon \cos E(t))^2}$, and the relation $\frac{dE}{dt} = \frac{1}{1-\varepsilon \cos E}$ (which in turn follows from taking the time derivative of the standard Kepler's equation $M = E - \varepsilon \sin E$; see Bate et al. (1971)).

6.2.2 Computational Results

In Figure 6, we show a 2D projection of an example globalized stable manifold mesh for a 5:6 Jupiter-Europa PERTBP invariant circle. This was computed using the regularized PERTBP equations of motion to evaluate F^{-k} in the procedure described in Section 6.1; in this case, $N = 2048$, $L = 101$, $k_{max} = 6$. We have

Fig. 6 (x, y) projection of Jupiter-Europa PERTBP 5:6 W^s for $\omega = 1.030011437$

filtered the computed mesh points so as to only plot those which did not result in a very "visually discontinuous" mesh; this filtering is needed during visualization, since close flybys of m_2 can send points which started close together in extremely different directions. Nevertheless, even after discarding some mesh points, it is clearly visible in the figure that the manifold passes through the singularity at m_2 (Europa, marked as a red circle). Using the regularized equations, we experienced no warnings of integrator divergence during program runtime, which were encountered when using the unregularized equations.

We also used the regularized equations of motion to recompute the 3:4 W^s manifold mesh shown earlier in Figure 5. The results matched those which were obtained earlier when using Eq. (3) and (5) for the numerical integrations, thus verifying the correctness of the regularization procedure. We carried out this computation in Julia, using the DP5 integrator and parallelizing across θ_i with the EnsembleProblem feature of DifferentialEquations.jl (Rackauckas and Nie 2017); the computation of the 3:4 manifold with $N = 1024$, $L = 101$, $k_{max} = 15$ took approximately 250 seconds on the same quad core i7 laptop CPU used earlier.

7 Conclusion

In this paper, we first developed a quasi-Newton method for the simultaneous computation of unstable invariant circles and their symplectic conjugate center, stable, and unstable bundles for stroboscopic maps of periodically-perturbed PCRTBP models. Our method improves the computational complexity of the torus calculation to $O(N \log N)$ as compared to $O(N^3)$ for the methods generally used in the existing literature, in addition to giving useful information on the stable and unstable directions. We used this quasi-Newton method for continuation of tori and bundles by both perturbation parameter and rotation number, and described how to initialize the continuation from PCRTBP periodic orbits. We also gave a set of numerical best practices to aid in quasi-Newton method convergence.

After finding the tori and bundles, we used the results of the continuation to start an order-by-order method for the computation of Fourier-Taylor series parameterizations of stable and unstable manifolds for the invariant circles. We found significant improvements in accuracy and fundamental domain size compared to linear manifold approximations. Finally, we were able to extend the parameterizations to compute points of the manifolds outside the fundamental domain, with the aid of a modified Levi-Civita regularization which we derived for the PERTBP. We expect that similar methods can be used to regularize other periodically-perturbed PCRTBP models as well.

The tools developed were tested in the Jupiter-Europa PERTBP, with the calculations of the circles, bundles, and manifold parameterizations taking just a few seconds on a 2017-era laptop with a quad-core Intel i7 CPU. Our Julia program for computation of meshes of globalized manifold points took a few minutes for each manifold, due to the large number of numerical integrations involved. As we describe in another paper (Kumar et al. 2021b), with the help of modern computer graphics processing units, these manifold parameterizations and meshes can be used to very rapidly search for and accurately compute intersections of stable and unstable manifolds leading to heteroclinic connections. The methods presented in this paper can form an important component for low-energy mission design and transfer trajectories in such periodically-perturbed PCRTBP models.

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