Semi-geostrophic particle motion and exponentially accurate normal forms

Colin J Cotter* Sebastian Reich†

February 7, 2013

Abstract

We give an exponentially-accurate normal form for a Lagrangian particle moving in a rotating shallow-water system in the semi-geostrophic limit, which describes the motion in the region of an exponentially-accurate slow manifold (a region of phase space for which dynamics on the fast scale are exponentially small in the Rossby number). We show how this result is related to the variational asymptotics approach of [**?**]; the difference being that on the Hamiltonian side it is possible to obtain strong bounds on the growth of fast motion away from (but near to) the slow manifold.

Our normal form approach extends to numerical approximations *via* backward error analysis, and extends to particle methods for the shallow-water equations, where the result shows that particles stay close to balance over long times in the semi-geostrophic limit.

1 Introduction

Semi-geostrophic approximations are obtained from the rotating shallow-water equations in the low Rossby and Burger number limit. In [**?**], a systematic approach for deriving these models is set out, based on looking for a near-identity change of coordinates for the solution domain which makes the Lagrangian affine (linear in velocity), resulting in a equation which only has slow dynamics. At each order in the Rossby number, there is some choice of parameters available, and this choice can be crucial in obtaining a well-posed PDE. After the change of coordinates, the equations of motion can be obtained by applying Hamilton's variational principle to the approximated Lagrangian.

In this paper we use exponentially-accurate normal form theory to investigate the rotating shallow-water equations in the limit of low Rossby and low Burger number. Exponentially-accurate normal form theory was first popularised through the work of [**?**] (very clearly reviewed and reformulated in [**?**]) on perturbed integrable Hamiltonian ODEs. Also important in the literature, [**?**] gave an exponentially-accurate estimate for systems with rapidly rotating phase, and [**?**] developed estimates for highly oscillatory mechanical systems. A first application of exponentially-accurate normal form transformations in the context of geophysical fluid dynamics can be found in [**?**]. The principle analytic obstruction to a result in our case is the requirement that the free surface height remains sufficiently smooth; hence, we restrict our result to individual particle trajectories moving in a fluid with a specified free surface height (a problem which has applications in tracking advected tracer particles: see the summary for details), to toy ODE systems and to numerical solutions obtained with the Hamiltonian particle-mesh method for the rotating shallow-water equations. The central tool of the normal form theory is the choice of a suitable symplectic transformation for the particle positions and momenta (this transformation may be more general than the cotangent-lifted coordinate transformations used in [**?**]), resulting in a Hamiltonian system where the small coupling between fast and slow time-scales is more explicit. More explicitly, if the model equations

*Department of Mathematics, Imperial College London, London SW7 2AZ, England, (e-mail: colin.cotter@imperial.ac.uk)

†Institut für Mathematik, Universität Potsdam, Postfach 60 15 53, D-14415 Potsdam, Germany (e-mail:sreich@math.uni-potsdam.de)

are solved with initial conditions which are close to balance, then they will stay there for very long time intervals. We also note that our results are more general than the type provided in [**?**], where the existence of a slow manifold up to exponentially small terms is shown.

The rest of the paper is organised as follows. In section 2 we introduce the model system of a particle moving in a rapidly-rotating shallow-water flow, and discuss the ideas behind geostrophy and semi-geostrophic approximations. In section 2.1 we introduce the variational structure of these equations from both of the Lagrangian and Hamiltonian viewpoints, and in section 2.2 we discuss higher-order balanced models in the context of the variational structure. This background then allows us to introduce the exponentially-accurate normal form theory in section 2.3, and we show how this theory extends to numerical solutions obtained with symplectic time-stepping methods in section 2.5. Section 3 applies this theory to particle methods for the rotating shallow-water equations. Section 3.1 discusses geostrophic balance for these methods in the context of exponentially-accurate normal form theory, whilst section 3.2 illustrates the theory with some numerical results. Finally there is a summary and outlook in section 4.

2 A model system

The shallow-water equations (SWEs) on an f-plane are

$$\begin{aligned} \frac{Du}{Dt} &= +fv - g\mu_x, && (1)\\ \frac{Dv}{Dt} &= -fu - g\mu_y, && (2)\\ \frac{D\mu}{Dt} &= -\mu\left(u_x + v_y\right). && (3) \end{aligned}$$

Here $\mu = \mu(t,x,y)$ is the fluid depth, g is the gravitational constant, f is twice the (constant) angular velocity of the reference plane,

$$\frac{D}{Dt}(.) = (.)_t + u(.)_x + v(.)_y, \tag{4}$$

is the Lagrangian or material time derivative, and subscripts denote partial differentiation with respect to that variable. See [**?**] for a derivation of the SWEs and their relevance to geophysical fluid dynamics.

In non-dimensionalised variables, the SWEs can be written in the form

$$\begin{aligned} \mathrm{Ro}\frac{Du}{Dt} &= +v - \frac{\mathrm{B}}{\mathrm{Ro}}\mu_x, && (5)\\ \mathrm{Ro}\frac{Dv}{Dt} &= -u - \frac{\mathrm{B}}{\mathrm{Ro}}\mu_y, && (6)\\ \frac{D\mu}{Dt} &= -\mu\left(u_x + v_y\right), && (7) \end{aligned}$$

where $\mathrm{Ro} = U/fL$ is the Rossby number and $\mathrm{B} = (L_R/L)^2$ is the Burger number. Furthermore, $L_R = \sqrt{gH}/f$ is the Rossby radius of deformation, U is a typical advection velocity, L is a typical length scale, and H is the mean fluid depth for the problem under consideration. Semi-geostrophic theory is concerned with the limit of (5)-(7) with $\mathrm{Ro} = \mathcal{O}(\varepsilon)$, $\mathrm{B} = \mathcal{O}(\varepsilon)$ as $\varepsilon \to 0$. For simplicity, we use $\mathrm{Ro} = \mathrm{B} = \varepsilon$ from now on. See [**?**] for a derivation of non-dimensionalised equations and the semi-geostrophic scaling limit.

Instead of investigating the full SWEs, we start in this paper with the following simpler model problem. We assume that the layer depth $\mu(\varepsilon t, x, y)$ is a given function of time t and space $\mathbf{x} = (x,y)^T$. We may then investigate the motion of a single fluid parcel with coordinates $\mathbf{q} = (q_x, q_y)^T$. The corresponding Newtonian equations of motion are given by

$$\varepsilon\frac{d^2 q_x}{dt^2} = +\frac{dq_y}{dt} - \mu_{q_x}(\varepsilon t, q_x, q_y), \tag{8}$$

$$\varepsilon \frac{d^2 q_y}{dt^2} = -\frac{dq_x}{dt} - \mu_{q_y}(\varepsilon t, q_x, q_y), \tag{9}$$

We next rescale time and introduce the new time-scale $\tau = \varepsilon\, t$. We denote time derivatives with respect to τ by overdot, *e.g.*, $dq_x/d\tau = \dot{q}_x$. We also write the second order equations (8)-(9) as a system of first order equations by introducing the momentum $\mathbf{p} = (p_x, p_y)^T$, *i.e.*,

$$\begin{aligned}
\dot{p}_x &= +p_y - \varepsilon\, \mu_{q_x}(\tau, q_x, q_y), && (10)\\
\dot{p}_y &= -p_x - \varepsilon\, \mu_{q_y}(\tau, q_x, q_y), && (11)\\
\dot{q}_x &= p_x, && (12)\\
\dot{q}_y &= p_y. && (13)
\end{aligned}$$

These equations may be expressed in a more compact form:

$$\begin{aligned}
\dot{\mathbf{p}} &= J_2\mathbf{p} - \varepsilon\, \nabla_{\mathbf{q}}\mu(\tau, \mathbf{q}), \qquad J_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, && (14)\\
\dot{\mathbf{q}} &= \mathbf{p}, && (15)
\end{aligned}$$

which is the formulation we will work with in this paper. A discussion of the relationship between the Hamiltonian structure of this system and the Hamiltonian structure for the full SWEs is given in [**?**].

The intuitive idea behind the semi-geostrophic approximation [**?**] is that the solutions of (14)-(15) consist of inertial oscillations with period $T_I = 2\pi = \mathcal{O}(\varepsilon^0)$ and slow geostrophically balanced motion on a (slow) time-scale $T_G = \mathcal{O}(\varepsilon)$. Furthermore, intuition suggests that the inertial oscillations are primarily governed by the linear equations

$$\begin{aligned}
\dot{\mathbf{p}} &= J_2\mathbf{p}, && (16)\\
\dot{\mathbf{q}} &= \mathbf{p}, && (17)
\end{aligned}$$

while the slow, geostrophically balanced, parcel dynamics is characterised by the reduced (nonlinear) system

$$\begin{aligned}
\mathbf{0} &= J_2\mathbf{p} - \varepsilon\, \nabla_{\mathbf{q}}\mu(\tau, \mathbf{q}), && (18)\\
\dot{\mathbf{q}} &= \mathbf{p}, && (19)
\end{aligned}$$

or, equivalently,

$$\dot{\mathbf{q}} = -\varepsilon\, J_2 \nabla_{\mathbf{q}}\mu(\tau, \mathbf{q}). \tag{20}$$

2.1 Hamiltonian and variational formulations

We start with a Hamiltonian formulation of the system (14)-(15). As a further simplification we assume that the layer-depth μ is time-independent and introduce the potential energy function $V(\mathbf{q}) := \mu(\mathbf{q})$ to make the link to classical mechanics more transparent.

We rewrite the equations (14)-(15) using a non-canonical symplectic structure operator

$$J = \begin{pmatrix} J_2 & -I_2 \\ I_2 & 0_2 \end{pmatrix} \in \mathbb{R}^{4\times 4}, \tag{21}$$

so that

$$\dot{\mathbf{z}} = J\nabla_{\mathbf{z}} H_0(\mathbf{z}), \tag{22}$$

with Hamiltonian

$$H_0(\mathbf{z}) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}), \quad K(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbf{p}, \tag{23}$$

and phase space variable $\mathbf{z} = (\mathbf{p}^T, \mathbf{q}^T)^T \in \mathbb{R}^4$.

Another approach is to rewrite the system of first-order equations as a second-order equation

$$\ddot{\mathbf{q}} - J_2\dot{\mathbf{q}} + \varepsilon \nabla_{\mathbf{q}} V(\mathbf{q}) = \mathbf{0}, \tag{24}$$

and to note that (24) is the Euler-Lagrange equation for the Lagrangian functional

$$\mathcal{L} = \int d\tau \left[\frac{1}{2} \|\dot{\mathbf{q}}\|^2 + \frac{1}{2} \mathbf{q}^T J_2 \dot{\mathbf{q}} - \varepsilon V(\mathbf{q}) \right]. \tag{25}$$

The reduced model (20) with $\mu = V$ is also Hamiltonian with phase space $\mathbf{q} \in \mathbb{R}^2$, structure matrix J_2^T, and Hamiltonian function $H_g(\mathbf{q}) = \varepsilon V(\mathbf{q})$. The associated Lagrangian functional is given by

$$\mathcal{L}_{\mathrm{g}} = \int d\tau \left[\frac{1}{2} \mathbf{q}^T J_2 \dot{\mathbf{q}} - \varepsilon V(\mathbf{q}) \right]. \tag{26}$$

Note that (26) differs from (25) by the missing kinetic energy term $\|\dot{\mathbf{q}}\|^2/2$.

2.2 Higher order balance and the 'semi-geostrophic' approximation

Clearly, one would like to derive more sophisticated reduced models; a systematic approach has recently been given in [**?**]. In this section we summarize the main results from [**?**] before we develop our novel approach in section 2.3.

All known derivations of balanced (semi-geostrophic) models start from the assumption that

$$\dot{\mathbf{q}} = -\varepsilon J_2 \nabla_{\mathbf{q}} V(\mathbf{q}) + \mathcal{O}(\varepsilon^2) = \mathcal{O}(\varepsilon). \tag{27}$$

Under this assumption, we may formally collect terms of equal order in ε and rewrite (25) as

$$\mathcal{L} = \varepsilon \int d\tau \left[L_0 + \varepsilon L_1 \right], \quad \text{where} \quad L_0 = \frac{1}{2\varepsilon} \mathbf{q}^T J_2 \dot{\mathbf{q}} - V(\mathbf{q}), \quad L_1 = \frac{1}{2\varepsilon^2} \|\dot{\mathbf{q}}\|^2. \tag{28}$$

We now introduce a coordinate transformation $\psi_\varepsilon : \mathbb{R}^2 \to \mathbb{R}^2$ and transformed coordinates $\mathbf{q}_\varepsilon$ via

$$\mathbf{q} = \psi_\varepsilon(\mathbf{q}_\varepsilon) = \mathbf{q}_\varepsilon + \varepsilon \mathbf{F}_1(\mathbf{q}_\varepsilon) + \mathcal{O}(\varepsilon^2). \tag{29}$$

Following [**?**] (but note our different notation), we set

$$\mathbf{F}_1(\mathbf{q}_\varepsilon) = -\frac{1}{2} \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) + \lambda \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) = -\frac{1}{2\varepsilon} J_2 \dot{\mathbf{q}}_\varepsilon + \lambda \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) + \mathcal{O}(\varepsilon). \tag{30}$$

Hence we obtain a Lagrangian function

$$\mathcal{L}_1 = \varepsilon \int d\tau \left[\bar{L}_0 + \varepsilon \bar{L}_1 + \mathcal{O}(\varepsilon^2) \right] \tag{31}$$

in the transformed variable $\mathbf{q}_\varepsilon$, where

$$\bar{L}_0 = \frac{1}{2\varepsilon} \mathbf{q}_\varepsilon^T J_2 \dot{\mathbf{q}}_\varepsilon - V(\mathbf{q}_\varepsilon), \qquad \bar{L}_1 = \varepsilon^{-1} \left[\frac{1}{2} + \lambda \right] \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)^T J_2 \dot{\mathbf{q}}_\varepsilon - \lambda \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2. \tag{32}$$

Upon dropping $\mathcal{O}(\varepsilon^3)$ terms in (31), we finally obtain the transformed Lagrangian

$$\mathcal{L}_1 = \int d\tau \left[\frac{1}{2} \mathbf{q}_\varepsilon^T J_2 \dot{\mathbf{q}}_\varepsilon - \varepsilon V(\mathbf{q}_\varepsilon) + \varepsilon \left[\frac{1}{2} + \lambda \right] \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)^T J_2 \dot{\mathbf{q}}_\varepsilon - \varepsilon^2 \lambda \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2 \right]. \tag{33}$$

In the context of this paper, the choice $\lambda = -1/2$ is of particular interest. Note that this choice corresponds to Salmon's large-scale semi-geostrophic approximation (see [**?**, **?**]). The associated reduced equations of motion can be derived from the Lagrangian functional

$$\mathcal{L}_{\mathrm{lsg}} = \int d\tau \left[\frac{\varepsilon^2}{2} \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2 + \frac{1}{2} \mathbf{q}_\varepsilon^T J_2 \dot{\mathbf{q}}_\varepsilon - \varepsilon V(\mathbf{q}_\varepsilon) \right]. \tag{34}$$

The associated Euler-Lagrange equations are explicitly given by

$$J_2 \dot{\mathbf{q}}_\varepsilon - \varepsilon \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) + \frac{\varepsilon^2}{2} \nabla_{\mathbf{q}} \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2 = \mathbf{0}. \tag{35}$$

These equations are canonical with Hamiltonian

$$H_{\rm lsg}(\mathbf{q}_\varepsilon) = \varepsilon V(\mathbf{q}_\varepsilon) - \frac{\varepsilon^2}{2}\|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2, \tag{36}$$

and structure matrix $J_{\rm lsg} = J_2^T$.

A number of questions arises at this stage.

1. The assumption (27) is essential for the derivation of the reduced Lagrangian (31). However, even if (27) holds at the initial time, how can one ensure that it holds true for solutions of the full equations (24) over finite (or infinite) time intervals?

2. Following [**?**], one can formally generalize the coordinate transformation to obtain higher-order balanced equations. Can this process be continued to arbitrary precision and what rigorous error bounds in terms of ε can be obtained?

3. What role is played by the parameter λ?

We will provide an answer to these questions from the perspective of Hamiltonian perturbation theory in the following sections. We will first restrict the discussion to the simple model system (14)-(15) before considering a generalization to particle methods for the SWEs in section 3.

We also wish to point the reader to the reports [**?**, **?**], which attempt to answer the above questions based on higher-order coordinate transformations

$$\mathbf{q}_\varepsilon = \mathbf{q} + \varepsilon \mathbf{F}_1 + \varepsilon^2 \mathbf{F}_2 + \cdots + \varepsilon^m \mathbf{F}_m + \mathcal{O}(\varepsilon^{m+1}) \tag{37}$$

and associated higher-order expansions

$$\mathcal{L}_m = \varepsilon \int d\tau \left[\bar{L}_0 + \varepsilon \bar{L}_1 + \cdots + \varepsilon^m \bar{L}_m + \mathcal{O}(\varepsilon^{m+1})\right] \tag{38}$$

of the Lagrangian functional for $m \geq 1$.

2.3 Exponentially accurate normal forms

In this section we view the finite dimensional system (22) from the Hamiltonian side and look for symplectic coordinate transformations to a normal form.

The precise aim of the normal form transformation is to find a symplectic (with respect to the structure matrix J) change of coordinates, which transforms the system to a form in which the fast and slow variables are completely separated up to a small remainder term. As the transformation is symplectic, the equations of motion can be obtained simply by substituting the change of coordinates into the Hamiltonian and writing down Hamilton's equations. This normal form strategy is well-developed and we only summarise the main steps. See, *e.g.*, [**?**] for the first derivation of an exponential estimate and [**?**] for an application to systems of type (22).

Our aim is to find a near-identity change of coordinates Ψ_n so that

$$H_n = H_0 \circ \Psi_n = K + \varepsilon G_n + \varepsilon^{n+1} R_n, \tag{39}$$

where

$$\{G_n, K\} = 0, \tag{40}$$

with $\{\cdot,\cdot\}$ being the Poisson bracket obtained from J.

We define Ψ_{n+1} recursively by writing

$$\Psi_{n+1} = \Psi_n \circ \Phi_{1,\varepsilon^{n+1}F_{n+1}}, \quad \Psi_0 = \mathrm{Id}, \tag{41}$$

where $\Phi_{1,\varepsilon^{n+1}F_{n+1}}$ is the time-1 flow map of the Hamiltonian vector field produced by the Hamiltonian function $H = \varepsilon^{n+1}F_{n+1}$. Recursive substitution gives

$$H_{n+1} = H_n \circ \Phi_{1,\varepsilon^{n+1}F_{n+1}} = K + \varepsilon G_n + \varepsilon^{n+1}(R_n + \{K, F_{n+1}\}) + \mathcal{O}(\varepsilon^{n+2}), \tag{42}$$

and so we need to choose F_{n+1} so that

$$R_n + \{K, F_{n+1}\} = \bar{R}_n, \tag{43}$$

where

$$\{\bar{R}_n, K\} = 0. \tag{44}$$

Equation (43) is known as the *homological equation*. The solution F_{n+1}, and the *non-resonant part* $\bar{R}_n$ of R_n can be calculated *via*

$$\bar{R}_n = \frac{1}{T}\int_0^T d\tau\, R_n \circ \Phi_{\tau,K}, \tag{45}$$

$$F_{n+1} = \frac{1}{T}\int_0^T d\tau\, \tau(R_n - \bar{R}_n) \circ \Phi_{\tau,K}, \tag{46}$$

where $\Phi_{\tau,K}$ is the time-τ flow-map of the Hamiltonian vector field produced by K, which is time-periodic with period $T = 2\pi$. To close the recursion we define

$$G_{n+1} = G_n + \varepsilon^n \bar{R}_n \tag{47}$$

and terms of size $\mathcal{O}(\varepsilon^{n+2})$ and smaller are collected in a new residual function R_{n+1}.

When the potential V is analytic and bounded on an appropriate compact set in the complex plane, we can choose to make the number of iterations scale with $1/\varepsilon$ and obtain an exponentially-accurate normal form as summarised in the following theorem:

Theorem 2.1. *Let $\mathscr{K}$ be some compact subset of phase space containing the solution trajectory, and let V be analytic in $B_r\mathscr{K}$ (the union of complex balls of radius r with centres in $\mathscr{K}$). Then there exists a near-identity change of coordinates Ψ_ε such that*

$$\tilde{H} = H_0 \circ \Psi_\varepsilon = K + \varepsilon\, G + e^{-c/\varepsilon}\, R, \tag{48}$$

where

$$\{G, K\} = 0, \tag{49}$$

G and R have ϵ-independent bounds on $\mathscr{K}$ and $c > 0$ is some constant.

Proof. Essentially the method is to obtain a Cauchy estimate for each remainder R_n, and to truncate the above algorithm after n steps where n scales with $1/\varepsilon$. Defining the norm on functions

$$|f|_r = \sup_{\boldsymbol{z}\in B_r\mathscr{K}} |f(\boldsymbol{z})|, \tag{50}$$

we obtain iterative estimates for $\bar{R}_n$ and F_{n+1} from equations (45-46) [**?**]:

$$|\bar{R}_n|_r \le |R_n|_r, \qquad |F_{n+1}|_r \le 2\pi |R_n|_r. \tag{51}$$

Simple adding and subtracting of terms gives

$$\begin{aligned} H_n \circ \Phi_{1,\epsilon^{n+1}F_{n+1}} &= K + [\epsilon G_n + \epsilon^{n+1}\{K, F_{n+1}\} + \epsilon^{n+1} R_n] \\ &\quad + K \circ \Phi_{1,\epsilon^{n+1}F_{n+1}} - K - \epsilon^{n+1}\{K, F_{n+1}\} \\ &\quad + \epsilon(G_n \circ \Phi_{1,\epsilon^{n+1}F_{n+1}} - G_n) \\ &\quad + \epsilon^{n+1}(R_n \circ \Phi_{1,\epsilon^{n+1}F_{n+1}} - R_n). \end{aligned} \tag{52}$$

The term in the square brackets is ϵG_{n+1}, and it remains to estimate this term, and the remainder. If we choose δ so that $r - (n+1)\delta > 0$ and H_n is analytic in $B_{r-n\delta}\mathcal{K}$ then

$$\begin{aligned} |G_{n+1}|_{r-(n+1)\delta} &= |G_n + \epsilon^n \overline{R}_n|_{r-(n+1)\delta}, \\ &\le |G_n|_{r-n\delta} + \epsilon^n |R_n|_{r-n\delta}, \end{aligned} \tag{53}$$

having used the estimate for $\overline{R}_n$. Estimates for the remainder R_{n+1} can be obtained using the mean-value theorem combined with a Cauchy estimate for the gradient. To estimate the second line in equation (52) note that

$$\begin{aligned}
& \mathcal{K}\circ\Phi_{1,\epsilon^{n+1}F_{n+1}} - \mathcal{K} - \epsilon^{n+1}\{\mathcal{K}, g_{n+1}\} \\
= \;& \epsilon^{n+1}\int_0^1 \{\mathcal{K}, F_{n+1}\}\circ\Phi_{t,\epsilon^{n+1}F_{n+1}}\,dt - \epsilon^{n+1}\{\mathcal{K}, F_{n+1}\}, \\
= \;& \epsilon^{n+1}\int_0^1 \{\mathcal{K}, F_{n+1}\}\circ\Phi_{t,\epsilon^{n+1}F_{n+1}} - \{\mathcal{K}, F_{n+1}\}dt, \\
= \;& \epsilon^{n+1}\int_0^1 (\overline{R}_n - R_n)\circ\Phi_{t,\epsilon^{n+1}F_{n+1}} - (\overline{R}_n - R_n)dt, \qquad (54)
\end{aligned}$$

which may be bounded using the mean-value theorem and a Cauchy estimate by

$$\begin{aligned}
& |\mathcal{K}\circ\Phi_{1,\epsilon^{n+1}F_{n+1}} - \mathcal{K} - \epsilon^{n+1}\{\mathcal{K}, g_{n+1}\}|_{r-(n+1)\delta} \\
\leq \;& \epsilon^{n+1}\int_0^1 \left|(\overline{R}_n - R_n)\circ\Phi_{t,\epsilon^{n+1}F_{n+1}} - (\overline{R}_n - R_n)\right|_{r-(n+1)\delta} dt, \\
\leq \;& \epsilon^{2(n+1)}|\nabla(\overline{R}_n - R_n)|_{r-(n+1)\delta}|F_{n+1}|_{r-(n+1)\delta} \\
\leq \;& \frac{2\pi\epsilon^{2(n+1)}}{\delta}|\overline{R}_n - R_n|_{r-n\delta}|R_n|_{r-(n+1)\delta}, \\
\leq \;& \frac{2\pi\epsilon^{2(n+1)}}{\delta}|R_n|_{r-n\delta}|R_n|_{r-n\delta}. \qquad (55)
\end{aligned}$$

Similar estimates give

$$\epsilon|G_n\circ\Phi_{1,\epsilon^{n+1}F_{n+1}} - G_n|_{r-(n+1)\delta} \leq \frac{2\pi\epsilon^{n+2}}{\delta}|G_n|_{r-n\delta}|R_n|_{r-n\delta}, \qquad (56)$$

$$\epsilon^{n+1}|R_n\circ\Phi_{1,\epsilon^{n+1}F_{n+1}} - R_n|_{r-(n+1)\delta} \leq \frac{2\pi\epsilon^{2(n+1)}}{\delta}|R_n|_{r-n\delta}|R_n|_{r-n\delta}. \qquad (57)$$

Suppose we have:

$$|G_n|_{r-n\delta} \leq c_0\sum_{i=1}^{n}\left(\frac{c_1\epsilon}{\delta}\right)^i, \quad |R_n|_{r-n\delta} \leq c_0\left(\frac{c_1}{\delta}\right)^n, \qquad (58)$$

where c_0 is a positive constant, and $c_1 = 4\pi c_0$, then we get

$$|G_{n+1}|_{r-(n+1)\delta} \leq c_0\sum_{i=1}^{n+1}\left(\frac{c_1\epsilon}{\delta}\right)^i, \qquad (59)$$

from equation (53), and

$$\begin{aligned}
|R_{n+1}|_{r-(n+1)\delta} &= \frac{2\pi\epsilon^{n+1}}{\delta}|R_n|_{r-n\delta}|R_n|_{r-n\delta} + \frac{2\pi}{\delta}|G_n|_{r-n\delta}|R_n|_{r-n\delta} \\
&\quad + \frac{2\pi\epsilon^{n+1}}{\delta}|R_n|_{r-n\delta}|R_n|_{r-n\delta}, \\
&\leq c_0\left(\frac{c_1}{\delta}\right)^n\left(\frac{4\pi\epsilon^{n+1}}{\delta}c_0\left(\frac{c_1}{\delta}\right)^n + \frac{2\pi}{\delta}c_0\sum_{i=1}^{n}\left(\frac{c_1\epsilon}{\delta}\right)^i\right), \qquad (60)
\end{aligned}$$

from equations (55-57). If

$$\frac{c_1\epsilon}{\delta} < \frac{1}{2}, \qquad (61)$$

then $|G_{n+1}|_{r-(n_1)\delta} \leq c_0$, and

$$|R_{n+1}|_{r-(n+1)\delta} \leq c_0\left(\frac{c_1}{\delta}\right)^n\frac{2\pi c_0}{\delta}\left(2\epsilon\frac{1}{2^n}+1\right) \leq c_0\left(\frac{c_1}{\delta}\right)^{n+1}. \qquad (62)$$

These estimates are true for all n by induction if we set $c_0 = |V|_r$. Finally we choose n to scale with ϵ from the formula

$$n = \left[\frac{2r}{ec_1\epsilon}\right] \tag{63}$$

where the square brackets indicate rounding up to the nearest integer, and set $\delta = r/2n$. Equation (61) can then be satisfied, and we get

$$\epsilon^{n+1}|R_n|_{r/2} \leq \epsilon c_0(\frac{\epsilon c_1}{\delta})^n \leq \epsilon c_0 \left(\frac{1}{e}\right)^{2/ec_1\epsilon} = \epsilon c_0 e^{-c\epsilon} \tag{64}$$

where $c = ec_1/2$. □

Let us denote the transformed variables by $\mathbf{z}_\varepsilon = (\mathbf{p}_\varepsilon^T, \mathbf{q}_\varepsilon^T)^T$. The transformed variables are defined by $\Psi_\varepsilon(\mathbf{z}_\varepsilon) = \mathbf{z}$. We can then obtain an estimate for $K(\mathbf{p}_\varepsilon(\tau))$ in these coordinates by

$$\begin{aligned} |K(\mathbf{p}_\varepsilon(\tau)) - K(\mathbf{p}_\varepsilon(0))| &< |\tau|\left|\frac{d}{d\tau}K(\mathbf{p}_\varepsilon(\tau))\right|, \\ &< |\tau||\{K, \tilde{H}\}|, \\ &< |\tau|e^{-c/\varepsilon}|\{K, R\}|, \\ &< de^{-c/2\varepsilon}, \end{aligned} \tag{65}$$

for $|\tau| < e^{c/2\varepsilon}$ and some constant $d > 0$. This means that $\|\mathbf{p}_\varepsilon(\tau)\|^2$ stays almost constant for very long time intervals.

Corollary 2.2. *Let us assume that the momenta* $\mathbf{p} = \dot{\mathbf{q}}$ *satisfy*

$$\mathbf{p}(0) = -\varepsilon J_2 \nabla_{\mathbf{q}} V(\mathbf{q}(0)) + \mathcal{O}(\varepsilon^2) \tag{66}$$

at initial time $\tau = 0$*, then*

$$\mathbf{p}(\tau) = -\varepsilon J_2 \nabla_{\mathbf{q}} V(\mathbf{q}(\tau)) + \mathcal{O}(\varepsilon^2) \tag{67}$$

for all $|\tau| < e^{c/2\varepsilon}$*.*

Proof. To first order in ε the slow manifold is determined by $\mathbf{p} = -\varepsilon J_2 \nabla_{\mathbf{q}} V(\mathbf{q})$ and, in terms of the transformed coordinates, by $\mathbf{p}_\varepsilon = \mathcal{O}(\varepsilon^2)$. Hence (66) implies that $K(\mathbf{p}_\varepsilon(0)) = \mathcal{O}(\varepsilon^4)$. Finally (65) yields the desired result. □

This means that provided the system is within $\mathcal{O}(\varepsilon^2)$ of the geostrophically balanced state initially, it will stay there for exponentially long time intervals. It is *not* necessary for the system to be exactly geostrophically balanced for the the result to hold.

If $\mathbf{p}_\varepsilon(0) = 0$, (*i.e.*, we start on the slow manifold) then there are no rapid oscillations due to $\mathbf{p}_\varepsilon$, and we get the symplectic slow equation given in the following corollary:

Corollary 2.3. *If* $\mathbf{p}_\varepsilon(0) = 0$ *then*

$$J_2 \dot{\mathbf{q}}_\varepsilon = \varepsilon \nabla_{\mathbf{q}} G(\mathbf{0}, \mathbf{q}_\varepsilon) + \mathcal{O}(e^{-c/2\varepsilon}), \tag{68}$$

for all $|\tau| < e^{c/2\varepsilon}$*.*

Proof. If $\mathbf{p}_\varepsilon(0) = 0$, then theorem 2.1 says that $\mathbf{p}_\varepsilon(t)$ stays exponentially small for exponentially long time intervals and so

$$\dot{\mathbf{q}}_\varepsilon = \varepsilon\, \nabla_{\mathbf{p}} G(\mathbf{p}_\varepsilon, \mathbf{q}_\varepsilon)|_{\mathbf{p}_\varepsilon = \mathbf{0}} + \mathcal{O}(e^{-c/2\varepsilon}), \tag{69}$$

for all $|\tau| < e^{c/2\varepsilon}$. We can obtain the slow equations in symplectic form by examining the $\mathbf{p}_\varepsilon$ equation and ignoring exponentially small terms, *i.e.*,

$$\mathbf{0} = \dot{\mathbf{p}}_\varepsilon = J_2 \nabla_{\mathbf{p}} G(\mathbf{p}_\varepsilon, \mathbf{q}_\varepsilon)|_{\mathbf{p}_\varepsilon = \mathbf{0}} - \nabla_{\mathbf{q}} G(\mathbf{p}_\varepsilon, \mathbf{q}_\varepsilon)|_{\mathbf{p}_\varepsilon = \mathbf{0}}, \tag{70}$$

and then substituting equation (69) to make

$$J_2 \dot{\mathbf{q}}_\varepsilon = \varepsilon \nabla_{\mathbf{q}} G(\mathbf{p}_\varepsilon, \mathbf{q}_\varepsilon)|_{\mathbf{p}_\varepsilon = 0} = \varepsilon \nabla_{\mathbf{q}} G(\mathbf{0}, \mathbf{q}_\varepsilon), \tag{71}$$

up to terms exponentially small in ε. □

We note that (68) is in canonical form, *i.e.*, the equations are Hamiltonian with structure matrix $J_{\rm lsg} = J_2^T$ and Hamiltonian $\hat{H}_{\rm lsg}(\mathbf{q}_\varepsilon) = \varepsilon\, G(\mathbf{0}, \mathbf{q}_\varepsilon)$. When the system is *not* initialised on the slow manifold then the dynamics is dominated by this slow equation but also contains fast components (which remain approximately of the same magnitude for exponentially long time intervals).

In section 2.6 we will conduct a simple experiment that will allow us to verify the above estimates numerically. The particular set-up will be chosen such that $\mathbf{p} = \mathbf{p}_\varepsilon$ at the initial time $\tau = 0$ and final time $\tau = T$. Then $|K(\mathbf{p}(0)) - K(\mathbf{p}(T))|$ should go to zero exponentially fast as $\varepsilon \to 0$ (discounting numerical round-off errors). We will show in section 2.5 that such exponentially small terms can indeed be observed using a symplectic time stepping method (see, *e.g.*, [**?**, **?**] for a discussion of symplectic time stepping methods for Hamiltonian ODEs).

In the appendix we calculate the slow equation (68) to second-order by applying the iterative algorithm and obtain

$$J_2 \dot{\mathbf{q}}_\varepsilon = \varepsilon \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) - \frac{\varepsilon^2}{2} \nabla_{\mathbf{q}} \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2 + \mathcal{O}(\varepsilon^3). \tag{72}$$

Note that the significant terms in (72) are equivalent to the 'large-scale semi-geostrophic' equation (35). In other words, (68) provides a higher order generalisation of the 'large-scale semi-geostrophic' theory in the context of our simple model system. More precisely, Hamiltonian normal form theory naturally leads to $\lambda = -1/2$.

2.4 Extension to non-autonomous systems

To recover results for equations (8)-(9) we need to extend the results from section 2.3 to systems with time-dependent potentials where the Hamiltonian takes the form

$$H_0(\mathbf{z}, \tau) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}, \tau). \tag{73}$$

We apply the standard technique of extending the phase space by two extra conjugate variables s and e, and write a new Hamiltonian

$$\bar{H}_0(\mathbf{z}, e, s, \tau) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}, s) - e, \tag{74}$$

so that the equations of motion for e and s are

$$\dot{s} = 1, \qquad \dot{e} = \varepsilon \frac{\partial V}{\partial s}(\mathbf{q}, s), \tag{75}$$

and we recover the original equations. The new Hamiltonian $\bar{H}_0$ is now autonomous and in a suitable form to apply theorem 2.1 with minor modifications (to account for the two extra variables), *i.e.*, there exists a near-identity symplectic change of coordinates $(\mathbf{p}, \mathbf{q}, e, s) \to (\mathbf{p}_\varepsilon, \mathbf{q}_\varepsilon, e_\varepsilon, s_\varepsilon)$ such that $K(\mathbf{p}_\varepsilon)$ is nearly preserved over exponentially long time intervals.

We will make use of this extension to non-autonomous systems again in section 3.2.

2.5 Numerical methods and backward error analysis

The Hamiltonian equations (14)-(15) can be solved numerically using a symplectic method. As an example, we give the following splitting method. We rewrite the Hamiltonian (23) as a sum

$$H_0 = \frac{1}{2} K + \varepsilon V + \frac{1}{2} K \tag{76}$$

and note that each entry has an exact flow map, which we denote by $\Phi_{\tau, K/2}$ and $\Phi_{\tau, \varepsilon V}$, respectively. A second-order symplectic method is now given by the composition of these flow maps [**?**], *i.e.*,

$$\mathbf{z}^{n+1} = M_{\Delta\tau}(\mathbf{z}^n), \qquad M_{\Delta\tau} = \Phi_{\Delta\tau/2, K} \circ \Phi_{\Delta\tau, \varepsilon V} \circ \Phi_{\Delta\tau/2, K}. \tag{77}$$

Using backward error analysis, it can be shown that this method is equivalent to the exact solution of a modified Hamiltonian problem up to terms exponentially small in $\Delta\tau$ [**?**, **?**]. More specifically, there exists a modified Hamiltonian

$$H_{\Delta\tau}(\mathbf{z}) = H_0(\mathbf{z}) + \varepsilon\,\Delta\tau^2 P(\mathbf{z}, \Delta\tau) \tag{78}$$

such that

$$\|M_{\Delta\tau}(\mathbf{z}) - \Phi_{\Delta\tau, H_{\Delta\tau}}(\mathbf{z})\| \leq c_1\, e^{-c_2/\Delta\tau}, \tag{79}$$

where $c_1, c_2 > 0$ are appropriate constants. See [**?**, **?**] for a survey of backward error analysis results for Hamiltonian systems.

The modified Hamiltonian (78) allows us to discuss the preservation of geostrophic balance under the time-stepping method (77). All one has to do is to apply the normal form transformation from the previous section to the modified Hamiltonian (78) and to generalise theorem 2.1. In particular, the following theorem implies the near conservation of geostrophic balance under the numerical method (77) over exponentially long times.

Theorem 2.4. *Consider a symplectic integrator*

$$\mathbf{z}^{n+1} = M_{\Delta t}(\mathbf{z}^n), \qquad \mathbf{z}^n = ((\mathbf{q}^n)^T, (\mathbf{p}^n)^T)^T, \tag{80}$$

such as (77). Then, for a sufficiently small time step $\Delta\tau$, there exists a symplectic change of coordinates $\Psi_{\varepsilon,\Delta\tau}$ such that

$$\|\Psi^{-1}_{\varepsilon,\Delta\tau} \circ M_{\Delta\tau} \circ \Psi_{\varepsilon,\Delta\tau}\,(\mathbf{z}_\varepsilon) - \Phi_{\Delta\tau, \tilde{H}_{\Delta\tau}}(\mathbf{z}_\varepsilon)\| < d_1\, e^{-d_2/\Delta\tau} \tag{81}$$

where $\mathbf{z}_\varepsilon = \Psi^{-1}_{\varepsilon,\Delta\tau}(\mathbf{z})$ denotes the transformed variable, $\Phi_{\tau,\tilde{H}_{\Delta\tau}}$ is the exact flow map of a Hamiltonian system with transformed Hamiltonian

$$\tilde{H}_{\Delta\tau} = H_{\Delta\tau} \circ \Psi_{\varepsilon,\Delta\tau} = K + \varepsilon G_{\Delta\tau} + e^{-d_3/\varepsilon} R_{\Delta\tau}, \tag{82}$$

*$H_{\Delta\tau}$ is the exponentially accurate modified Hamiltonian for $M_{\Delta t}$ (*i.e.*, (79) holds), and $d_i > 0$, $i = 1, 2, 3$, are appropriate constants. The transformation is chosen such that*

$$\{K, G_{\Delta\tau}\} = 0. \tag{83}$$

Furthermore, as $\Delta\tau \to 0$,

$$G_{\Delta\tau} \to G, \qquad R_{\Delta\tau} \to R, \tag{84}$$

where G and R are given in theorem 2.1.

Proof. The proof combines normal form estimates with backward error analysis for symplectic methods as developed in [**?**] for adiabatic invariants in highly oscillatory mechanical systems. In particular, backward error analysis implies that the trajectory of the symplectic method $M_{\Delta\tau}$ stays $\Delta\tau$-exponentially close to the exact solution of a system with a modified Hamiltonian $H_{\Delta\tau}$ consisting of H_0 perturbed by an $\mathcal{O}(\varepsilon\Delta\tau^p)$ correction, $p \geq 1$ the order of the method. We then apply theorem 2.1 to the modified Hamiltonian $H_{\Delta\tau}$. □

Theorem 2.4 implies that if $\mathbf{p}^0$ is initialised at zero in the transformed coordinates, then $\mathbf{p}^n$ will stay exponentially close to zero in the transformed coordinates over exponentially long times. This statement agrees with general results on the preservation of adiabatic invariants under symplectic time-stepping methods. See, for example, [**?**] and [**?**]. We will make use of this property of symplectic methods in the following section.

Another immediate (more practical) conclusion from theorem 2.4 is the following

Corollary 2.5. *Numerical trajectories computed with a symplectic method such as (77) satisfy*

$$\mathbf{p}^n = -\varepsilon J_2 \nabla_{\mathbf{q}} V(\mathbf{q}^n) + \mathcal{O}(\varepsilon^2), \tag{85}$$

over exponentially many time-steps n provided the conditions of theorem 2.4 are satisfied and (85) holds at $n = 0$.

Proof. The proof is similar to that of corollary 2.2. □

2.6 A numerical experiment

We consider the particular potential energy function

$$V(\mathbf{q}) = q_x + \frac{1}{2}\exp(-(q_x^2 + q_y^2)), \qquad \mathbf{q} = (q_x, q_y)^T, \tag{86}$$

and initial conditions

$$q_x(0) = 0, \quad q_y(0) < -10, \quad p_x(0) = 0, \quad p_y(0) = \varepsilon, \tag{87}$$

i.e., $V(\mathbf{q}(0)) \approx 0$. Simulations are run for long enough such that $q_y(T) > 10$ at final time T. The nonlinear dynamics reduces to a linear system

$$\dot{q}_x = 0, \qquad \dot{q}_y = \varepsilon \tag{88}$$

at both $\tau = 0$ and $\tau = T$, *i.e.*, to a system in perfect balance. More precisely, according to the theoretical results of sections 2.3 & 2.5, this statement should be true at final time up to terms exponentially small in ε.

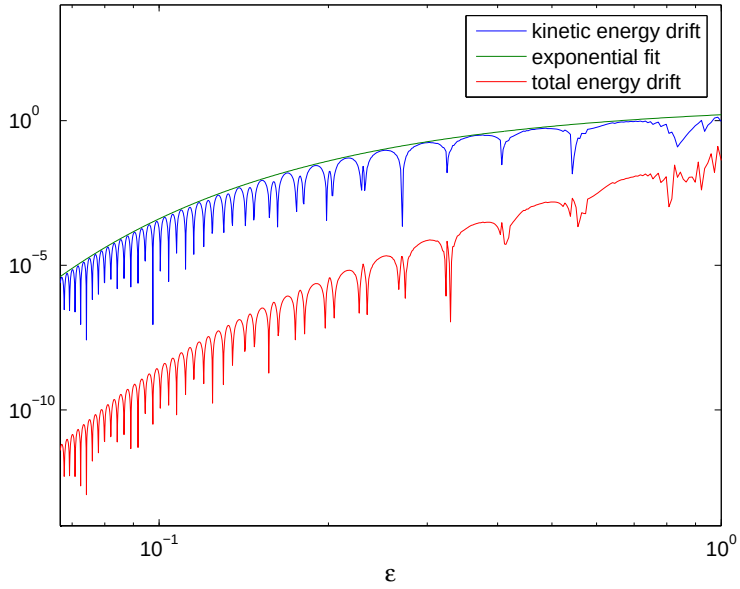

Figure 1: Drift in total energy, kinetic energy, and exponential fit with $4\exp(-0.92/\varepsilon)$ as a function of ε.

We conduct a numerical experiment to verify this claim. We implement the symplectic method (77) with step size $\Delta\tau = \varepsilon^2$ and vary ε in the interval $\tau \in [1/15, 1]$. The drift in total energy $\Delta E = |H(\mathbf{q}(0), \mathbf{p}(0)) - H(\mathbf{q}(T), \mathbf{p}(T))|$ and in kinetic energy $\Delta K = |K(\mathbf{p}(0)) - K(\mathbf{p}(T))|$ is monitored as a function of ε and the results are displayed in figure 1. The drift in total energy is solely caused by the symplectic time stepping method. The choice of $\Delta\tau$ ensures that this drift is orders of magnitude smaller than the computed drift in kinetic energy. In other words, finite step size effects on the generation of unbalanced motion can be neglected. The anticipated exponential dependence of the drift in kinetic energy is nicely confirmed and

$$\Delta K \leq 4\,\exp(-0.92/\varepsilon) \tag{89}$$

provides an excellent bound confirming theorem 2.4 with $d_3 = 0.92$.

3 Particle methods for the shallow-water equations

Throughout section 2, we have assumed that the fluid depth μ is a given function of space and time and derived equations of motion for a single 'fluid parcel'. In this section, we consider a numerical approximation for μ of the form

$$\mu(t,\mathbf{x}) = \sum_{i=1}^{N} m_i\, \psi(\|\mathbf{x}-\mathbf{q}_i(t)\|) \tag{90}$$

in terms of N moving 'fluid parcels', where $\mathbf{q}_i(t) \in \mathbb{R}^2$ denotes the location of the ith fluid parcel at time t with mass m_i and shape function $\psi(r) \geq 0$. The approximation (90) provides the typical starting point for a particle method such as smoothed particle hydrodynamics (SPH), which was first proposed in [**?**, **?**] for general fluid dynamics and for the SWEs (1)-(3) in [**?**].

Each 'fluid parcel' moves under the Newtonian equations of motion

$$\begin{aligned} \mathrm{Ro}\frac{d}{dt}\mathbf{p}_i &= J_2\mathbf{p}_i - \frac{\mathrm{B}}{\mathrm{Ro}}\nabla_{\mathbf{x}}\mu(t,\mathbf{x})|_{\mathbf{x}=\mathbf{q}_i}, & (91)\\ \frac{d}{dt}\mathbf{q}_i &= \mathbf{p}_i & (92) \end{aligned}$$

The equations (90)-(92) form a closed set of equations and provide an approximation to (5)-(7). (See [**?**, **?**, **?**, **?**] for a numerically robust implementation of a particle method for the SWEs and their geometric properties.)

After setting $\mathrm{B} = \mathrm{Ro} = \varepsilon$ and a rescaling of time, equations (91)-(92) become

$$\begin{aligned} \dot{\mathbf{p}}_i &= J_2\mathbf{p}_i - \varepsilon\nabla_{\mathbf{x}}\mu(\mathbf{x},t)|_{\mathbf{x}=\mathbf{q}_i}, & (93)\\ \dot{\mathbf{q}}_i &= \mathbf{p}_i. & (94) \end{aligned}$$

Without restriction of generality, we may also assume that all 'fluid parcels' carry a constant mass $m_i = \delta$. The equations (90), (93)-(94) are Hamiltonian with Hamiltonian function

$$H_{\mathrm{sph}}(\mathbf{z}) = K(\mathbf{p}) + \varepsilon V(\mathbf{q}) = \sum_{i=1}^{N}\frac{1}{2}\|\mathbf{p}_i\|^2 + \frac{\varepsilon\,\delta}{2}\sum_{i,j}^{N}\psi(\|\mathbf{q}_i-\mathbf{q}_j\|), \tag{95}$$

structure matrix

$$J = \begin{pmatrix} J_{2N} & -I_{2N} \\ I_{2N} & 0_{2N} \end{pmatrix} \in \mathbb{R}^{2N\times 2N}, \tag{96}$$

phase space variable $\mathbf{z} = (\mathbf{q}^T, \mathbf{p}^T)^T \in \mathbb{R}^{4N}$, and $\mathbf{q} = (\mathbf{q}_1^T, \ldots, \mathbf{q}_N^T)^T$, $\mathbf{p} = (\mathbf{p}_1^T, \ldots, \mathbf{p}_N^T)^T$. Note that a finite fluid depth μ implies that the particle masses $m_i = \delta$ approach zero as the number of particles $N \to \infty$. More precisely, $\delta\, N \approx \mathit{const.}$ as $N \to \infty$.

3.1 Preservation of geostrophic motion

We first note that the Hamiltonian system defined by (95)-(96) with $N = 1$ fits exactly into the framework of section 2. Furthermore, as first observed in [**?**], the normal form theory developed in section 2 can be generalised to $N > 1$ without much difficulty. The key idea goes back to an observation in [**?**]. Specifically, it turns out that the normal form theory for a system with many degrees of motion with identical fast frequency proceeds much along the lines of the theory for a single fast degree of motion. Most importantly, the exponential estimates do not depend on the number of degrees of freedom and we obtain:

Theorem 3.1. *We consider a fixed number of particles N. Let the shape function ψ be analytic in some compact subset of $\mathbb{C}^{2N}$ containing the solution trajectory. Then there exists a near-identity change of coordinates Ψ_ε such that*

$$\tilde{H} = H_{\mathrm{sph}} \circ \Psi_\varepsilon = K + \varepsilon\, G + e^{-c/\varepsilon}\, R \tag{97}$$

where

$$\{G, K\} = 0 \tag{98}$$

and $c > 0$ *is some constant.*

Proof. We apply theorem 2.1 in slightly modified form taking into account that $N > 1$. We also note that a bound on ψ immediately implies a bound on the potential energy V *via* $|V(\mathbf{q})| \leq \delta N |\psi|_\infty$. □

The estimate (65) hence also applies to the particle approximation (93)-(94) and geostrophic balance is maintained over exponentially long time intervals. Furthermore, theorem 2.4 and corollary 2.5 immediately carry over to the particle method. Note that (85) gets replaced by

$$\mathbf{p}_i^n = -\varepsilon J_2 \nabla_{\mathbf{x}} \mu(\mathbf{x}, t)|_{\mathbf{x}=\mathbf{q}_i} + \mathcal{O}(\varepsilon^2) \tag{99}$$

for $i = 1, \ldots, N$. Recall that we consider the limit $\varepsilon \to 0$ for N fixed.

It is important to keep in mind that theorem 3.1 does *not* apply to most practical implementations of particle method since the basis functions are typically not analytic. In those case the exponentially small term in (97) needs to be replaced by a polynomial expression of the form $(c\varepsilon)^k$, where the integer $k \geq 2$ and the constant $c > 0$ depend on the smoothness of the basis function ψ. This is the case, for example, for the Hamiltonian-Particle-Mesh (HPM) method (see [**?**]), which will be used in the following section to conduct a number of numerical experiments.

3.2 Numerical experiments

In this section, two numerical examples are given which illustrates theorems 2.4 and 3.1 for practical implementations of a particle method.

3.2.1 Exchange of kinetic energy

To show that particles may exchange energy as long as the total kinetic energy is preserved, consider a model consisting of 2 interacting particles moving on a predefined background height field $\overline{\mu}(\tau, \boldsymbol{x})$. In this experiment, we use the Hamiltonian Particle-Mesh (HPM) method for spatial discretisation (see [**?**]) with the total fluid depth at a grid point $\mathbf{x}_{mn}$ given by

$$\mu_{mn}(\tau) = \sum_{i=1}^{2} \psi_{mn}(\mathbf{q}_i(\tau)) + \overline{\mu}(\tau, \mathbf{x}_{mn}). \tag{100}$$

The basis functions ψ_{mn} are normalized cubic B-splines centered about grid points $\mathbf{x}_{mn}$.

We multiplied the potential energy by an analytic function $g(\tau)$ with $g(\tau) \to 0$ as $\tau \to \pm\infty$ so that the Hamiltonian takes the form

$$H_{\mathrm{hpm}}(\mathbf{z}) = \sum_{i=1}^{2} \frac{1}{2} \|\mathbf{p}_i\|^2 + \frac{\varepsilon}{2} g(\tau) \sum_{mn} \sum_{i=1}^{2} \psi_{mn}(\mathbf{q}_i) \left(\sum_{j=1}^{2} \psi_{mn}(\mathbf{q}_j) + 2\overline{\mu}(\tau, \mathbf{x}_{mn}) \right). \tag{101}$$

The reason for the introduction of the function $g(\tau)$ is that when $g(\tau) \approx 0$ at the beginning and the end of the simulation, the Hamiltonian is already in normal form and we can measure the amount of fast rotational energy exactly (this technique was first introduced in [**?**] in an experiment to measure the exchange of oscillatory energy between two colliding molecules).

A graph showing kinetic energy against time during the experiment, and a plot of the trajectories of the two particles is shown in figure 2. This example illustrates that, although the total kinetic energy K is almost invariant, the particles exchange energy through the interaction potential as shown in figure 3. This exchange is permitted because the frequencies of oscillation of the two particles are the same for $\varepsilon = 0$.

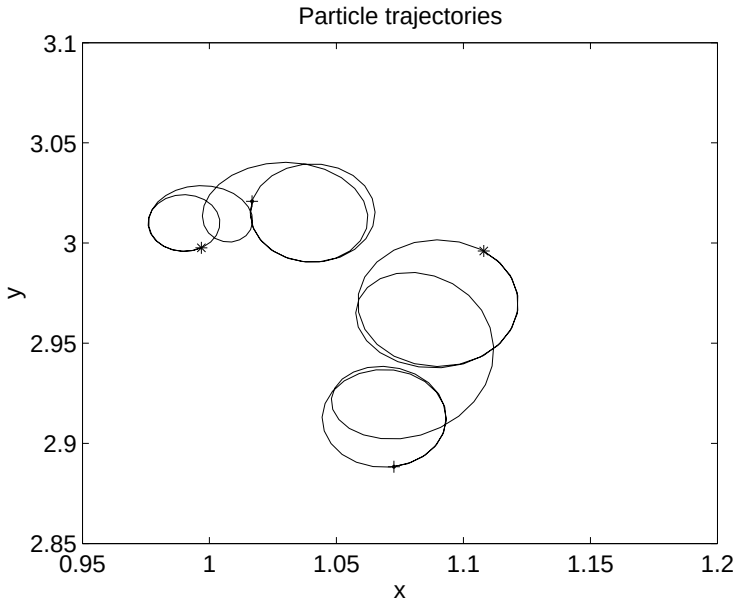

Figure 2: Plots showing particle trajectories for a system of 2 interacting HPM particles moving on a prescribed background height field. The initial positions are marked with a '*' and the end positions are marked with a '+'. The kinetic energy for each particle is shown in figure 3.

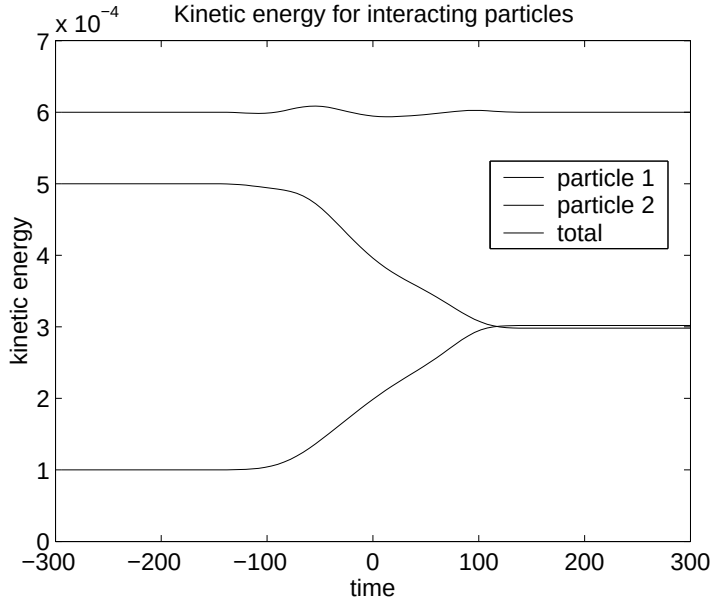

Figure 3: Plots showing kinetic energies for 2 interacting HPM particles moving on a prescribed background height field. The total kinetic energy returns at the end of the experiment to a value very close to the starting value. However the 2 particles do exchange kinetic energy.

3.2.2 Preservation of geostrophic balance under the HPM method

As already eluded to, theorem 3.1 does not directly apply to the HPM method [?] since the basis functions are not analytic. However, one would nevertheless expect 'good' preservation of geostrophic balance in the semi-geostrophic scaling limit. To test this hypothesis numerically, we repeated the shear flow instability simulation of [?] under slightly modified initial conditions such that the associated Rossby and Burger number satisfy Ro $\approx$ Bu ≈ 0.1. The HPM discretized shallow water equations are simulated using $N = 262144$ particles over a domain $(x, y) \in [0, 2\pi]^2$, a smoothing length of $\alpha = 0.2015$, and a time step of $\Delta t = 1/36$. Note that one unit of time corresponds to one day and that the Rossby radius of deformation corresponds to $L_R \approx 0.5$ in dimensionless variables. The initial momenta are in geostrophic balance, *i.e.*,

$$\mathbf{p}(0) = -\varepsilon J_{2N} \nabla_{\mathbf{q}} V(\mathbf{q}). \tag{102}$$

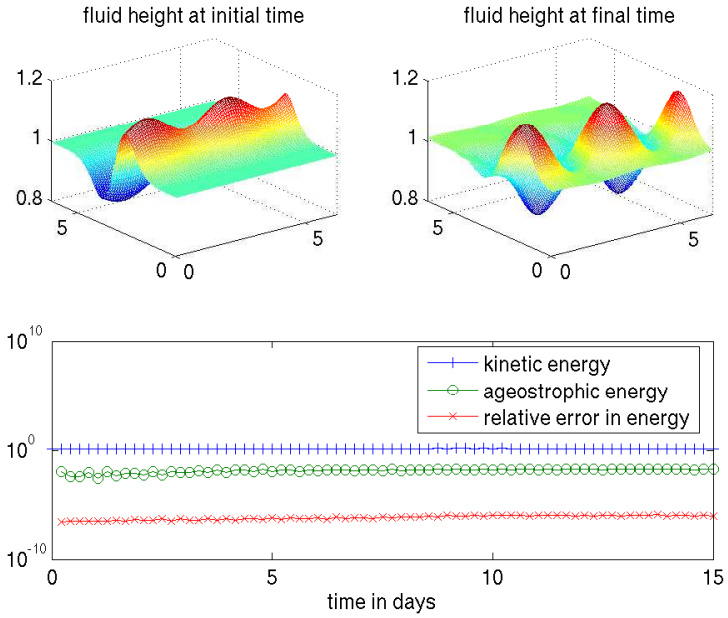

Figure 4: Drift in total energy, kinetic energy, and exponential fit with $4\exp(-0.92/\varepsilon)$ as a function of ε.

Simulation results can be found in figure 4, where we display the initial and final layer depth ($t = 15$ days). We also monitor the total kinetic energy $K(\mathbf{p})$, the total kinetic energy in the ageostrophic momentum components

$$\mathbf{p}_{\text{ag}} = \mathbf{p} - \mathbf{p}_{\text{gs}}, \qquad \mathbf{p}_{\text{gs}} = -\varepsilon J_{2N} \nabla_{\mathbf{q}} V(\mathbf{q}), \tag{103}$$

i.e., $K(\mathbf{p}_{\text{ag}})$, and the relative error in total energy H_{hpm}. We find that the relative error in energy remains very small. This is due to the symplectic nature of the time stepping procedure. We also observe that $K(\mathbf{p}_{\text{ag}})$ remains nearly level and much smaller than the kinetic energy $K(\mathbf{p})$. This indicates that geostrophic balance is well preserved throughout the simulation even though $\varepsilon \approx 0.1$ is not very small and the basis functions ψ_{mn} are not analytic.

4 Summary and outlook

We introduced the model system of a single fluid particle moving in a rotating shallow-water system and gave an exponentially-accurate normal form theorem valid in the semi-geostrophic scaling

limit. This normal form theorem gives a coordinate change for which the kinetic energy stays almost invariant for very long time intervals. When the kinetic energy in transformed variables is initially zero (or close to zero) we showed that it is possible to derive an exponentially-accurate slow equation which is equivalent to the symplectic slow equation obtained by variational asymptotics in the semi-geostrophic limit.

We showed that this result may be extended to numerical schemes for solving the SWEs based on particle methods by making use of backward error analysis, and then illustrated this with a numerical experiment designed to "capture" the exact amount of energy exchanged between the slow and fast dynamics.

The extension of this work to the full rotating shallow-water PDE (1)-(3) requires bounds to be obtained on the gradients of the height field. As the SWEs are known to develop shocks it seems unlikely that an exponentially-accurate result will be valid for long times unless it is possible to obtain some extra regularity when the fast dynamics has very little energy. It may be possible to obtain estimates for regularised equations where a smoothing operator is applied to the height gradient in the momentum equation, or for the family of α-regularised equations such as shallow-water-α [**?**].

Finally we suggest one possibly fruitful application of this work in the calculation of the dispersion of passive tracers using Lagrangian particles. Typically these calculations are performed by interpolating a given (gridded) velocity field $\mathbf{u}_{mn}(t)$ from the grid to the whole domain, and solving the system of ODEs

$$\frac{d\mathbf{q}_i}{dt} = \sum_{mn} \psi_{mn}(\mathbf{q}_i)\, \mathbf{u}_{mn}(t), \qquad i = 1, \ldots, N. \tag{104}$$

This method can often experience problems with artificial clumping of particles when the trajectories are integrated over long time intervals. An alternative approach would be to solve equations (8)-(9) with a given fluid depth (or geopotential) μ. The results of this paper show that if the system is integrated with a suitable symplectic method then the tracer particles will keep balanced trajectories in the semi-geostrophic limit.

Acknowledgement

We thank Georg Gottwald and Marcel Oliver for stimulating discussions on the relation of the Hamiltonian normal form theory, as proposed in [**?**], and the asymptotic variational approach of [**?**, **?**, **?**].

Appendix. Calculation of slow equation in symplectic form to second-order

In this appendix we explicitly calculate the change of coordinates and the slow equation to $\mathcal{O}(\epsilon^2)$ using the iterative procedure given in section 2.3.

The Hamiltonian vector field given by the kinetic energy $K = \|\mathbf{p}\|^2/2$ is

$$\dot{\mathbf{p}} = J_2\mathbf{p}, \qquad \dot{\mathbf{q}} = \mathbf{p},$$

and the associated time-τ flow map $\Phi_{\tau,K}$ is

$$\begin{aligned} \mathbf{p} &\mapsto e^{J_2\tau}\mathbf{p}, \\ \mathbf{q} &\mapsto J_2(1 - e^{J_2\tau})\mathbf{p} + \mathbf{q}. \end{aligned}$$

First we need to calculate the transformed Hamiltonian after the first-order transformation.

$$\begin{aligned} H_1 &= H_0 \circ \Phi_{1,\varepsilon F_1}, \\ &= H_0 + \varepsilon\{H_0, F_1\} + \frac{\varepsilon^2}{2}\{\{H_0, F_1\}, F_1\} + \mathcal{O}(\varepsilon^3), \end{aligned}$$

$$
\begin{aligned}
&= K + \varepsilon V + \varepsilon\{K, F_1\} + \varepsilon^2\{V, g_1\} + \frac{\varepsilon^2}{2}\{\{K, F_1\}, F_1\} + \mathcal{O}(\varepsilon^3),\\
&= K + \varepsilon\bar{V} + \frac{\varepsilon^2}{2}\{\bar{V} + V, F_1\} + \mathcal{O}(\varepsilon^3),
\end{aligned}
$$

where we have used $\{K, g_1\} = \bar{V} - V$, $\{K, \bar{V}\} = 0$, and

$$
\begin{aligned}
\bar{V}(\mathbf{z}) &= \frac{1}{T}\int_0^T d\tau\, V \circ \Phi_{\tau,K}(\mathbf{z}),\\
&= \frac{1}{T}\int_0^T d\tau\, V\left(J_2\left(1 - e^{J_2\tau}\right)\mathbf{p} + \mathbf{q}\right),
\end{aligned}
$$

as well as

$$
\begin{aligned}
F_1(\mathbf{z}) &= \frac{1}{T}\int_0^T d\tau\, \tau(V - \bar{V}) \circ \Phi_{\tau,K}(\mathbf{z}),\\
&= \frac{1}{T}\int_0^T d\tau\, \tau\left(V\left(J_2\left(1 - e^{J_2\tau}\right)\mathbf{p} + \mathbf{q}\right) - \int_0^T d\tau'\, V\left(J_2\left(1 - e^{J_2(\tau+\tau')}\right)\mathbf{p} + \mathbf{q}\right)\right).
\end{aligned}
$$

Recall that $\mathbf{z} = (\mathbf{p}^T, \mathbf{q}^T)^T$ and $T = 2\pi$.

The first-order slow equation is given by:

$$
J_2\dot{\mathbf{q}} = \varepsilon\nabla_{\mathbf{q}}\bar{V}\left(\mathbf{p}, \mathbf{q}\right)|_{\mathbf{p}=\mathbf{0}} = \varepsilon\nabla_{\mathbf{q}}V(\mathbf{q}).
$$

To calculate the slow equation at the next order, we write the transformed Hamiltonian after the first-order transformation as

$$
H_2 = K + \varepsilon\bar{V} + \varepsilon^2\bar{R}_1 + \mathcal{O}(\varepsilon^3),
$$

where

$$
R_1 = \frac{1}{2}\{\bar{V} + V, F_1\}.
$$

Note that for a general function $f(\mathbf{p}, \mathbf{q})$,

$$
\nabla_{\mathbf{q}}\bar{f}(\mathbf{p}, \mathbf{q})|_{\mathbf{p}=\mathbf{0}} = \frac{1}{T}\int_0^T d\tau\, \nabla_{\mathbf{q}}\left\{f\left(e^{J_2\tau}\mathbf{p}, J_2\left(1 - e^{J_2\tau}\right)\mathbf{p} + \mathbf{q}\right)\right\}|_{\mathbf{p}=\mathbf{0}} = \nabla_{\mathbf{q}}f(\mathbf{0}, \mathbf{q}),
$$

so all that remains is to calculate R_1 and the gradient with respect to $\mathbf{q}$ for $\mathbf{p} = \mathbf{0}$.

We have

$$
\{\bar{V}, F_1\} = \nabla_{\mathbf{p}}\bar{V} \cdot J_2\nabla_{\mathbf{p}}F_1 + \nabla_{\mathbf{q}}\bar{V} \cdot \nabla_{\mathbf{p}}F_1 - \nabla_{\mathbf{p}}\bar{V} \cdot \nabla_{\mathbf{q}}F_1,
$$

and

$$
\{V, F_1\} = \nabla_{\mathbf{q}}V \cdot \nabla_{\mathbf{p}}F_1.
$$

Now we need to calculate these various gradients:

$$
\begin{aligned}
\nabla_{\mathbf{q}}F_1(\mathbf{z})|_{\mathbf{p}=\mathbf{0}} &= \frac{1}{T}\int_0^T d\tau\, \tau\nabla_{\mathbf{q}}(V - \bar{V}) \circ \Phi_{\tau,K}(\mathbf{z})|_{\mathbf{p}=\mathbf{0}},\\
&= \nabla_{\mathbf{q}}(V(\mathbf{q}) - V(\mathbf{q})) = \mathbf{0},
\end{aligned}
$$

and

$$
\begin{aligned}
\nabla_{\mathbf{p}}F_1(\mathbf{z})|_{\mathbf{p}=\mathbf{0}} = \frac{1}{T}\int_0^T d\tau\, \tau\Bigg[&J_2\left(1 - e^{J_2\tau}\right)\nabla_{\mathbf{q}}V\left(J_2\left(1 - e^{J_2\tau}\right)\mathbf{p} + \mathbf{q}\right)|_{\mathbf{p}=\mathbf{0}} -\\
&\int_0^T d\tau'\, J_2\left(1 - e^{J_2(d\tau+d\tau')}\right)\nabla_{\mathbf{q}}V\left(J_2\left(1 - e^{J_2\tau}\right)\mathbf{p} + \mathbf{q}\right)|_{\mathbf{p}=\mathbf{0}}\Bigg],
\end{aligned}
$$

$$
\begin{aligned}
&= \left(\frac{-1}{T} \int_0^T d\tau\, \tau \left[J_2 \left(1 - e^{J_2 \tau}\right) - \int_0^T d\tau'\, J_2 \left(1 - e^{J_2 (d\tau + d\tau')}\right) \right] \right) \nabla_{\mathbf{q}} V(\mathbf{q}), \\
&= \left(\frac{1}{T} \int_0^T d\tau\, \tau \left[J_2 \left(1 - e^{J_2 \tau}\right) - J_2 \right] \right) \nabla_{\mathbf{q}} V(\mathbf{q}), \\
&= \frac{-1}{T} \int_0^T d\tau\, J_2 \tau e^{J_2 \tau} \nabla_{\mathbf{q}} V(\mathbf{q}), \\
&= \frac{-1}{T} \int_0^T d\tau\, \tau \frac{d}{d\tau} e^{J_2 \tau} \nabla_{\mathbf{q}} V(\mathbf{q}), \\
&= -\nabla_{\mathbf{q}} V(\mathbf{q}).
\end{aligned}
$$

We also obtain

$$
\begin{aligned}
\nabla_{\mathbf{q}} \bar{V}(\mathbf{z})|_{\mathbf{p}=\mathbf{0}} &= \frac{1}{T} \int_0^T d\tau\, \nabla_{\mathbf{q}} V \left(J_2 \left(1 - e^{J_2 \tau}\right) \mathbf{p} + \mathbf{q} \right))|_{\mathbf{p}=\mathbf{0}}, \\
&= \nabla_{\mathbf{q}} V(\mathbf{q}).
\end{aligned}
$$

and

$$
\begin{aligned}
\nabla_{\mathbf{p}} \bar{V}(\mathbf{z})|_{\mathbf{p}=\mathbf{0}} &= \frac{-1}{T} \int_0^T d\tau\, \left(1 - e^{-J_2 \tau}\right) J_2 \nabla_{\mathbf{q}} V \left(J_2 \left(1 - e^{J_2 \tau}\right) \mathbf{p} + \mathbf{q} \right) |_{\mathbf{p}=0}, \\
&= -J_2 \nabla_{\mathbf{q}} V(\mathbf{q}).
\end{aligned}
$$

Hence we get

$$
\{\bar{V}, F_1\}|_{\mathbf{p}=\mathbf{0}} = -\left(J_2 \nabla_{\mathbf{q}} V\right) \cdot \left(J_2 \nabla_{\mathbf{q}} V\right) - \nabla_{\mathbf{q}} V \cdot \nabla_{\mathbf{q}} V = 0,
$$

and

$$
\{V, F_1\}|_{\mathbf{p}=\mathbf{0}} = -\nabla_{\mathbf{q}} V \cdot \nabla_{\mathbf{q}} V = -\|\nabla_{\mathbf{q}} V\|^2,
$$

and so $R_1 = -\frac{1}{2} \|\nabla_{\mathbf{q}} V\|^2$. The slow equation in transformed coordinates is then

$$
J_2 \dot{\mathbf{q}}_\varepsilon = \varepsilon \nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon) - \frac{\varepsilon^2}{2} \nabla_{\mathbf{q}} \|\nabla_{\mathbf{q}} V(\mathbf{q}_\varepsilon)\|^2 + \mathcal{O}(\varepsilon^3).
$$

We note that this is the same slow canonical equation obtained using variational asymptotics in [**?**, **?**] and, in particular, yields the 'large-scale semi-geostrophic' equation (35).