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Conclusions

5.1 Main achieved results

The present work is devoted to the study of some bifurcations of plane Poiseuille flow. The main part is carried out by the full numerical integrator of the Navier–Stokes equations formulated in terms of velocity and pressure. It is described in sections 2.1–2.6. We have implemented two slightly different versions for the cases when the average flux or the mean pressure gradient through the channel are held constant. We have adopted a spectral discretization for spatial derivatives by means of Fourier series and Chebyshev polynomials for the stream and cross-stream variables respectively. A typical scheme in finite differences has been employed for the temporal discretization, whose precision has been checked using extrapolation methods for different initial conditions, Reynolds numbers, and discretizations: they proved the predicted theoretical order 2 of the method. Likewise, the reduction to one third of the original dimension as detailed in §2.4, has greatly increased the computation speed of the numerical integrator. We have applied dynamical system techniques, such as Poincaré sections and continuation methods, to the numerical integrator in order to obtain different flow configurations: time-periodic flows, tori of 2 and 3 frequencies, and more disordered solutions.

In chapter 3 we have solved an algebraic problem corresponding to the stationary version of the numerical integrator previously mentioned. According to the theoretical results of appendix A, these stationary flows in the appropriate Galilean reference are rotating waves. Using Re as a continuation parameter, by means of the results in §2.8, we traverse the curve of rotating waves for several values of the wavenumber α . The minimum values found for Re are in good agreement with those reported by Herbert (1976). No secondary two-dimensional flow were obtained for $Re_Q < 2594$ and $Re_p < 2934$. The stability of the rotating waves to disturbances with the same α has been carried out using the analytical linearization of the system of equations around the stationary solution. From the stability analysis we have detected several Hopf bifurcations on the upper branch of secondary flows. Numerical values for the first three Hopf bifurcations are reported in §3.4 for $\alpha = 1.1$ and $N \times 70$ for $N = 4, \dots, 8$ as the spatial discretization. As Herbert (1976) pointed out, we also found slow convergence of the Fourier series for secondary flows, as N is increased. This is one of the reasons for the disagreement between Soibelman & Meiron’s (1991) results and ours, together with the different formulation of the equations employed. Convergence

on the location of the Hopf bifurcations is better for the lower values of Re . In spite of this we have achieved similar qualitative results about the Hopf bifurcations as Soibelman & Meiron's (1991), in what concerns to their number and location on the upper branch of secondary flows.

We have computed the curve of periodic flows for $\alpha \in [0.75, 1.50]$, $Re_p \in [2900, 14000]$ and 4×40 as the spatial resolution. As a remarkable fact for $\alpha \approx 1$, is that the first Hopf bifurcation appears on the upper branch, meanwhile there is no stability change at the minimum Re_p of the curve. Up to $Re_p \approx 12000$ for $\alpha = 1.1$ we have only found two Hopf bifurcations. On the other hand for Re_Q , at the minimum point of the curve there is a stability change, which corresponds to a simple real eigenvalue crossing the imaginary axis and hence there is no bifurcating branch at this point. Further on the upper branch, for $Re_Q \approx 10000$, we have observed about 5 Hopf bifurcations in which a complex eigenvalue crosses the imaginary axis from negative real part to positive on increasing Re_Q . Unfortunately we have not achieved convergence in their values for $N \leq 8$. In the case of Re_p analogous bifurcations seem to occur for larger values of Re_p . But this analysis needs more number of nodes and it has not been carried out in the present work, since we are mainly interested in moderate values of Re .

Taking $\alpha = 1.1$, $\alpha = 1.02056$, 8×70 as the spatial resolution, and $\Delta t = 0.02$, we have analysed the unstable manifold of secondary flows with just one unstable real eigenvalue or two unstable complex conjugate eigenvalues. To this end, we first approach the unstable manifold by perturbing the rotating wave in the direction of the linear subspace associated to the unstable eigenvalue/s and then we follow the time evolution of the perturbed flow until it reaches a new attracting state. In the lower branch we have found secondary flows whose unstable manifold drives the fluid to the laminar flow, or to the periodic flow on the upper branch, or to a quasi-periodic flow, or even to more disordered configurations. We have detailed the different situations obtained in §3.5. On the contrary, the unstable manifold on the upper branch after the Hopf bifurcation is always connected with a 2-torus of the bifurcating family considered in chapter 4. This kind of instability is analogous to the situation mentioned by Chen & Joseph (1973), when disturbances of a stable laminar flow escape its domain of attraction, eventually snap through the unstable periodic solution and then are attracted by other flow with larger amplitude. The case of Re_p for $\alpha = 1.02056$ is qualitatively similar to Re_Q for $\alpha = 1.1$ as is shown in tables 3.15 and 3.16.

For the first two Hopf bifurcations of time-periodic flows, we have studied in chapter 4 the bifurcating branch of quasi-periodic flows in the case of Re_p and the first Hopf bifurcation for Re_Q . Quasi-periodic solutions are obtained as time-periodic flows in a suitable Galilean reference and this is numerically implemented as the search of fixed points of a Poincaré map. Again, by means of numerical continuation, we traverse the curve of quasi-periodic orbits as Re varies. The first Hopf bifurcation for constant pressure at Re_{p1} presents severe numerical restrictions originated by the instability of the quasi-periodic flows and by the large values of the return time τ to the considered Poincaré section. The best situation has minimum $\tau \approx 3000$ for $\alpha = 1.48$, meanwhile for $\alpha = 1.0$ it is $\tau \approx 10000$. Because the restrictions of long time integration, we have only been able to trace locally the curve of quasi-periodic solutions from Re_{p1} . The further we advanced in Re_p , the larger values of τ we encountered. Close to Re_{p1} and with the discretization employed ($N = 8$, $M = 70$, $\Delta t = 0.02$), it seems that we have achieved both qualitative and quantitative convergence. By observing figure 4.2 we can conjecture that, for the range of $\alpha \in [1, 1.1]$ considered, the minimum $Re \approx 2900$ attained with travelling waves is not lowered by quasi-periodic flows. This question still remains open for two-dimensional flows although Ehrenstein & Koch (1991) solved the gap between experiments and numerical results in the case

of three-dimensional flows.

Comparing Soibelman & Meiron's (1991) computations and ours, we find the main quantitative differences due to the larger number of Fourier modes we have taken, together with the distinct formulations of the Navier–Stokes equations employed. The important qualitative difference is the kind of bifurcation found at Re_{p1} : in their results (see §1.3 for a summary) this bifurcation is subcritical, but improving the precision of the numerical approach we obtain that it is supercritical. Then, the bifurcating quasi-periodic orbits that we have obtained are unstable. This has also been confirmed by numerical simulations.

For $Re_p > Re_{p2}$ the quasi-periodic flows encountered are attracting and the return time τ is of the order of tens, so in this case the computational cost is drastically reduced compared with the bifurcation at Re_{p1} . The range of Re_p traversed in the curve of attracting flows moves now to several thousands. However, in spite of keeping qualitative convergence, the use of larger Reynolds numbers, makes necessary an increase in spatial precision to get furthermore quantitative convergence. In the interval of Re_p analysed we have not detected any change of stability: bifurcated solutions at Re_{p1} are always unstable, meanwhile on the bifurcation at Re_{p2} they are stable to disturbances of the same wavelength.

When the flux is kept constant we have also analysed the first Hopf bifurcation at Re_{Q1} to quasi-periodic flows mainly for $\alpha = 1.1$. We have found the bifurcating branch of two-dimensional tori at the Hopf bifurcation. The located 2-tori are attracting up to $Re_Q \approx 7950$, considering only disturbances with the same wavenumber $\alpha = 1.1$. At this point the family of tori has a Hopf bifurcation changing to unstable solutions and giving rise to a family of attracting tori with 3 frequencies. As was mentioned in §1.3, Jiménez (1987) also obtained these families of attracting solutions for $\alpha = 1.0$, but not the unstable ones. We have not found unstable quasi-periodic solutions which bifurcate from Re_{p2} , but bearing in mind that the Hopf bifurcations of periodic flows occur for Re_p further away than for Re_Q and apparently in the same quantity, we can conjecture the instability of 2-tori at larger values of Re_p .

We have also analysed the unstable manifold of 2-tori for Re_Q and $\alpha = 1.1$. For $Re_Q \lesssim 9000$ this manifold is connected with 3-torus, but for greater Re_Q we have obtained other kind of apparently strange sets. The backward continuation of this strange sets have shown the existence of two different attracting flows for $Re_Q \approx 7800$: namely a 2-torus and an ordered but complicated solution.

Comparing the different configurations found for Re_p and Re_Q we can say that the kind of configurations for both settings are the same, namely, periodic flows, 2 and 3-tori and strange sets. The main qualitative differences are due to the existence of a first Hopf bifurcation for Re_p not present for Re_Q . For the range of Re considered, the kind of solutions detected for Re_Q also exists for a larger value of Re_p .

5.2 Limitations of the search method of quasi-periodic flows. Future work

The implemented approach to search quasi-periodic solutions is based on the numerical integrator of the Navier–Stokes equations developed in chapter 2. For this reason, at Re_{p1} we encounter great difficulties in the search of these flows. We have had to stop the search after a short interval of Re_p , because of the bad conditioning of the Jacobian matrix of the Poincaré map. At this limit

value of Re_p , very small variations of simply one coordinate of the initial flow, produces an image point of the Poincaré map very distant of the unperturbed flow. This implies a poorly estimated Jacobian matrix and hence divergence of Newton iterations. In addition, the instability of these solutions obstructs even more their search. A possibility to overcome this problem can be the application of a parallel shooting technique: The main idea consists of the split of the Poincaré map in several intermediate maps, say n , so the number of degrees of freedom is multiplied by $n + 1$, but the instability of the flow is reduced with shorter integration times. For the remaining Hopf bifurcations τ is substantially lower, what makes that, for the range of Re considered, this problem is not detected. We believe that this methodology can also be applied to similar problems.

As future work, it would be of interest the extension of the quasi-periodic flows found at Re_{p1} to a wide range of Re_p and their bifurcations, and analogously for the other considered bifurcations of Re_Q and Re_p to 2-tori and 3-tori; whether they bifurcate into other class of more complicated solutions: a new vortical state which could approach more the transition to turbulence. It is also of interest to consider disturbances of different wavelength, in order to confirm the stability of attracting solutions for a fixed wavelength. Finally, a challenging study is the transition problem in three dimensions and the stability of two-dimensional flows to three-dimensional disturbances, which has been considered in Orszag & Patera (1983*b*).

A

Appendix

Spatio-temporal symmetries

This appendix justifies the important reduction that allows periodic flows to be considered as stationary solutions if the observer moves in the stream direction at an adequate speed and, analogously, quasi-periodic flows behave as periodic for an appropriate speed of the observer. Those reductions are connected respectively with the approach adopted in the calculations of chapters 3 and 4. The results presented here are a modified and detailed version of some results of Rand (1982).

A.1 Generalities

Let H be a Hilbert space whose inner product $\langle \cdot, \cdot \rangle$ generates a norm $\| \cdot \|$ which has C^∞ dependence upon $v \in H - \{0\}$.

Definition A.1. A smooth semiflow φ on H is a one-parameter family of maps φ^t , for $t \geq 0$, whose domains are open subsets of H and which possess the following properties:

- The mapping $(t, v) \rightarrow \varphi^t(v)$ is defined on an open subset of $[0, \infty) \times H$ which contains $\{0\} \times H$ and is jointly continuous in t and v .
- For all $v \in H$, $\varphi^0(v) = v$. For all v in the domain of φ^{s+t} , $\varphi^{s+t}(v) = \varphi^s(\varphi^t(v))$.
- If K is a bounded subset of H and $\varphi^t(v)$ lies in K for all t for which $\varphi^t(v)$ is defined, then $\varphi^t(v)$ is defined for all $t \geq 0$.
- For all $t \geq 0$ the mapping φ^t is of class C^∞ .

The proof of the next theorem can be found in Marsden & McCracken (1976) p. 289.

Theorem A.2. The Navier–Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{Re} \Delta \mathbf{u},$$

on a compact Riemannian manifold M in dimension $d = 2$ or 3 , define a smooth semiflow on

$$H = \{ \mathbf{u} : M \rightarrow \mathbb{R}^d \mid \mathbf{u} \in W^{2,2}, \operatorname{div} \mathbf{u} = 0, \mathbf{u} = 0 \text{ on } \partial M \},$$

where $W^{2,2}$ is the Sobolev space of functions on M whose derivatives up to order 2 are in L_2 .

For the Poiseuille problem (1.5)–(1.6), we consider $M = [0, L] \times [-1, 1]$ identifying points $(0, y), (L, y) \in M$ in order to obtain periodic boundary conditions.

Definition A.3. Let Γ denote the circle group $\mathbb{R}/L\mathbb{Z}$. A representation of Γ on H is a homomorphism R of Γ into the group of continuous linear isomorphisms of H .

Thus if $\theta \in \Gamma$ we denote $R_\theta = R(\theta)$ as the continuous linear isomorphism on H defined by R . By definition, R must satisfy $R_0 = 1_H$ and $R_{\theta+\psi} = R_\theta \circ R_\psi$. We will also define for $v \in H$ its Γ -orbit and φ -orbit respectively as $O_\Gamma(v) = \{R_\theta(v) : \theta \in \Gamma\}$ and $O_\varphi(v) = \{\varphi^t(v) : t \geq 0\}$.

Definition A.4. A representation R of Γ on H is said to be continuous if for each $v \in H$, the map $\theta \mapsto R_\theta(v)$ is continuous.

For the case of Poiseuille problem, we define $R_\theta(\mathbf{u}(x, y, t)) = \mathbf{u}(x - \theta, y, t)$ as the representation of Γ on H . R_θ corresponds to a translation of θ in the observer's position in the stream direction. This is easily verified to be a continuous representation. Furthermore, since $\mathbf{u}(x - \theta, y, t)$ is a solution, provided this is so for $\mathbf{u}(x, y, t)$, then

$$R_\theta \varphi^t(\mathbf{u}(x, y, 0)) = \mathbf{u}(x - \theta, y, t) = \varphi^t(\mathbf{u}(x - \theta, y, 0)) = \varphi^t R_\theta(\mathbf{u}(x, y, 0)).$$

Hence the semiflow φ^t commutes with R for all $\theta \in \Gamma$, $\mathbf{u} \in H$ and t such that $\varphi^t(\mathbf{u})$ is defined. We will also use this hypothesis in the results of this appendix.

For $v \in H$ let

$$\begin{aligned} \Gamma(v) &= \{\theta \in \Gamma : R_\theta(v) = v\}, \\ Z^+(v) &= \{(t, \theta) \in [0, \infty) \times \Gamma : R_\theta(v) = \varphi^t(v)\}. \end{aligned}$$

$\Gamma(v) \subset \Gamma$ represents the spatial symmetries of v , meanwhile $Z^+(v)$ defines the spatio-temporal symmetries of v . We can consider $\Gamma(v) \subset Z^+(v)$ by identifying $\theta \in \Gamma$ with $(0, \theta) \in Z^+(v)$. We need the following lemmas.

Lemma A.5. If $C \subset \mathbb{R}$ is an additive subgroup of \mathbb{R} then $C = \tau\mathbb{Z}$ for some $\tau > 0$ or C is dense in \mathbb{R} .

Proof: See for instance Sotomayor (1979) p. 218. □

Lemma A.6. If $\Gamma(v) \neq \Gamma$ then $\Gamma(v) = (L/m)\mathbb{Z}$ for some $m \in \mathbb{Z}$.

Proof: It is immediate that $\Gamma(v)$ is a subgroup of Γ . We check that $\Gamma(v)$ is also closed. Let $\theta_n \rightarrow \theta$ as $n \rightarrow \infty$, such that $\theta_n \in \Gamma(v)$. Then, because R is continuous,

$$v = R_{\theta_n}(v) \xrightarrow{n \rightarrow \infty} R_\theta(v) = v,$$

and thus $\Gamma(v)$ is closed. Now applying lemma A.5 we obtain the result. □

A.2 Rotating waves

Lemma A.7. *If $Z^+(v) \neq \Gamma(v)$ then $v_t = \varphi^t(v)$ is defined for all $t \geq 0$ and has a unique extension to a solution defined for all $t \in \mathbb{R}$.*

Proof: Since $Z^+(v) \neq \Gamma(v)$, there exists $\tau > 0$ and $\theta \in \Gamma$ such that $v_\tau = \varphi^\tau(v) = R_\theta(v)$. For $s \in \mathbb{R}$ we put $s = n\tau + r$, for $n \in \mathbb{Z}$ and $0 \leq r < \tau$, and thus we define $w_s = R_{n\theta}\varphi^r(v)$. If for some $t \in \mathbb{R}$ there exists $v_t = \varphi^t(v)$, then writing $t = n\tau + r$, for $n \in \mathbb{Z}$ and $0 \leq r < \tau$, we have

$$w_t = R_{n\theta}\varphi^r(v) = \varphi^r R_{n\theta}(v) = \varphi^{n\tau+r}(v) = \varphi^t(v) = v_t.$$

Now considering the map

$$\begin{aligned} [0, L] \times [0, \tau] &\longrightarrow H \\ (\alpha, t) &\longmapsto R_\alpha(\varphi^t(v)), \end{aligned}$$

we have from hypothesis a) of definition A.1 and definition A.4 that it is continuous and therefore $K = \{R_\alpha(\varphi^t(v)) : (\alpha, t) \in [0, L] \times [0, \tau]\}$ is bounded. As $w_s \in K$ for every s , from hypothesis c) of definition A.1, we conclude that $v_t = w_t$ is defined for all $t \geq 0$. Finally, if v_t satisfies the evolution equation $dv/dt = X(v)$ for $t \geq 0$, then by means of the definition of derivative it is easy to verify that

$$\frac{dw}{dt}(t) = \lim_{h \rightarrow 0} \frac{w_{t+h} - w_t}{h} = X(w_t),$$

also for $t < 0$. By uniqueness of solutions we conclude that w_t is the unique extension of v_t defined for all $t \in \mathbb{R}$. \square

If $Z^+(v) \neq \Gamma(v)$ and w_t is the uniquely defined solution extending $v_t = \varphi^t(v)$ to $t \in \mathbb{R}$, then $Z^+(v)$ generates the subgroup $Z(v) = \{(t, \theta) \in \mathbb{R} \times \Gamma : w_t = R_\theta(w_0)\}$. If $Z^+(v) = \Gamma(v)$ then $Z^+(v)$ is a subgroup of $\mathbb{R} \times \Gamma$ which we also denote by $Z(v)$. In both cases the subgroup $Z(v)$ of $\mathbb{R} \times \Gamma$ is called the spatio-temporal symmetry group of v .

Lemma A.8. *If $v_{t_0} = \varphi^{t_0}(v)$ then $Z(v_{t_0}) = Z(v)$.*

Proof: Let us first suppose that there exists $s \neq 0$ such that $(s, \theta) \in Z(v)$, and consequently let w_t be the uniquely defined solution extending v_t , for which $w_s = R_\theta(v)$. Defining $\bar{w}_t = w_{t+t_0}$ for $t \in \mathbb{R}$, it turns out that \bar{w}_t is the unique extension of the solution $\varphi^t(v_{t_0})$. Because now φ^t is a flow, we can then write

$$\begin{aligned} (s, \theta) \in Z(v) &\iff w_s = R_\theta(v) \iff \varphi^{t_0}(w_s) = \varphi^{t_0}(R_\theta(v)) \\ &\iff \bar{w}_s = w_{s+t_0} = R_\theta(\varphi^{t_0}(v)) = R_\theta(v_{t_0}) \iff (s, \theta) \in Z(v_{t_0}). \end{aligned}$$

Thus, we have shown that if $Z^+(v) \neq \Gamma(v)$ then $Z(v_{t_0}) = Z(v)$. If $Z^+(v) = \Gamma(v)$, by uniqueness of solutions we have

$$\begin{aligned} \theta \in \Gamma(v_{t_0}) &\iff R_\theta(v_{t_0}) = v_{t_0} \iff \varphi^{t_0} R_\theta(v) = \varphi^{t_0}(v) \\ &\iff R_\theta(v) = v \iff \theta \in \Gamma(v), \end{aligned}$$

and again it is shown that $Z(v_{t_0}) = Z(v)$. \square

We introduce the lifts $\tilde{\Gamma}(v) = \{\theta \in \mathbb{R} : R_\theta(v) = v\}$ of $\Gamma(v)$ and $\tilde{Z}(v) = \{(t, \theta) \in \mathbb{R}^2 : R_\theta(v) = \varphi^t(v)\}$ of $Z(v)$, where R_θ stands for $R_\theta \bmod L$, convention we adopt henceforth.

Lemma A.9. a) If $O_\Gamma(v) = O_\varphi(v)$ and $\tilde{\Gamma}(v) = (L/m)\mathbb{Z}$, then for some $\alpha \in \mathbb{R}$, $\tilde{Z}(v) = \{(t, \theta) : \theta = \alpha t \bmod L/m\}$. b) If $O_\Gamma(v) \neq O_\varphi(v)$, $Z^+(v) \neq \Gamma(v)$ and $\tilde{\Gamma}(v) = (L/s)\mathbb{Z}$, then there exists $\tau > 0$ and $\Phi \in \mathbb{R}$ such that $\tilde{Z}(v) = \{(n\tau, n\Phi + Lp/s) : n, p \in \mathbb{Z}\}$.

Proof: a) Since $\tilde{\Gamma}(v) = (L/m)\mathbb{Z}$, then $O_\Gamma(v) = \{R_\theta(v) : \theta \in [0, L/m)\}$ and the map

$$\begin{aligned} R : [0, L/m) &\longrightarrow O_\Gamma(v) \\ \theta &\longmapsto R_\theta(v), \end{aligned}$$

is bijective and continuous by the hypothesis of definition A.4. Treating $[0, L/m)$ as a circle, we consider it as a compact set and thus $O_\Gamma(v)$ is also compact, so we conclude that R^{-1} is continuous. This fact allows us to define for each t where there exists $\varphi^t(v) \in O_\varphi(v) = O_\Gamma(v)$, a continuous function $\theta(t) = R^{-1}(\varphi^t(v)) \in [0, L/m)$ such that $\varphi^t(v) = R_{\theta(t)}(v)$. Hence $\theta(0) = 0$ and

$$R_{\theta(s+t)}(v) = \varphi^{s+t}(v) = \varphi^s(\varphi^t(v)) = \varphi^s(R_{\theta(t)}(v)) = R_{\theta(s)}(R_{\theta(t)}(v)) = R_{\theta(s)+\theta(t)}(v).$$

Bearing in mind that R is a bijection we obtain $\theta(s+t) = \theta(s) + \theta(t)$. From the linearity of $\theta(t)$ we may express $\theta(t) = \alpha t$ for $\alpha = \theta(1)$ and a) is proved.

b) From the hypothesis $O_\Gamma(v) \neq O_\varphi(v)$ and $Z^+(v) \neq \Gamma(v)$, there exists (τ, Φ) such that $\varphi^\tau(v) = R_\Phi(v)$ and $\varphi^t(v) \notin O_\Gamma(v)$ for $0 < t < \tau$, i.e. we select $\tau > 0$ as the minimum t for which $\varphi^t(v) = R_\Phi(v)$ for some $\Phi \in \mathbb{R}$. We consider now $(t, \theta) \in \tilde{Z}(v)$, so that $\varphi^t(v) = R_\theta(v)$. Taking $n \in \mathbb{Z}$ such that $0 < t + n\tau \leq \tau$, then $\varphi^{t+n\tau}(v) = R_{\theta+n\Phi}(v)$, so it must be $t + n\tau = \tau$ and $\theta + n\Phi = \Phi \bmod L/s$, or in other words $t = (1-n)\tau$, $\theta = (1-n)\Phi + Lp/s$ for $p \in \mathbb{Z}$. This proves b). \square

Definition A.10. A solution $v_t = \varphi^t(v)$ is called a rotating wave if $\tilde{Z}(v) = \{(t, \theta) : \theta = ct \bmod L/m\}$ for some $c \in \mathbb{R}$ and $m \in \mathbb{N}$.

Lemma A.11. If $v_t = \varphi^t(v)$ is a rotating wave with period T and $\tilde{\Gamma}(v) = (L/m)\mathbb{Z}$, then $v_t = R_{ct}(v)$ for $c = \pm LT/m$.

Proof: From definition A.10 $R_\theta(v) = \varphi^t(v)$ for $\theta = ct \bmod L/m$, $c \in \mathbb{R}$ and $m \in \mathbb{N}$. This implies $\varphi^t(v) = R_{ct}(v)$, provided $\tilde{\Gamma}(v) = (L/m)\mathbb{Z}$. On the other hand by the periodicity of v , $R_{cT}(v) = \varphi^T(v) = v$ and $R_{ct}(v) = \varphi^t(v) \neq v$ if $0 < t < T$. As a consequence $cT = \pm L/m$ and the result follows. \square

Theorem A.12. If for $v \in H$, $\Gamma(v) \neq \Gamma$ and $v_t = \varphi^t(v)$ is an isolated periodic solution of φ^t , then v_t is a rotating wave.

Proof: If $v_t = \varphi^t(v)$ is a periodic orbit of period, say T , then for all $\theta \in \Gamma$ one has $\varphi^T(R_\theta(v)) = R_\theta(\varphi^T(v)) = R_\theta(v)$ and therefore $\varphi^t(R_\theta(v))$ is also a periodic orbit. Since, as a function of θ , $R_\theta(v)$ is continuous and v_t is suppose to be an isolated periodic orbit, then $O_\Gamma(v) = O_\varphi(v)$ and applying a) of lemma A.9 the theorem is proved. \square

A.3 Modulated waves

Definition A.13. A solution $v_t = \varphi^t(v)$ is a modulated wave if $\tilde{\Gamma}(v) = (L/s)\mathbb{Z}$ for some $s \in \mathbb{N}$ and there exists $\tau > 0$ and $\Phi \in \mathbb{R}$ such that $\tilde{Z}(v) = \{(n\tau, n\Phi + Lp/s) : n, p \in \mathbb{Z}\}$. The vector (s, τ, Φ) is called the modulation data.

Theorem A.14. If v lies on an isolated invariant 2-torus \mathbb{T} , $\Gamma(v) \neq \Gamma$ and $v_t = \varphi^t(v)$ is not asymptotic to a rotating wave, then v_t is a modulated wave.

Proof: Since \mathbb{T} is an invariant 2-torus and R_θ is an automorphism for $\theta \in \Gamma$, $R_\theta\mathbb{T}$ is also an invariant 2-torus. The supposition of \mathbb{T} being isolated implies $R_\theta\mathbb{T} = \mathbb{T}$ for $\theta \in \Gamma$. Let $\mathbb{T}/\Gamma = \{O_\Gamma(v) : v \in \mathbb{T}\}$ denote all Γ -orbits in \mathbb{T} , endowed with the quotient topology. As $\Gamma(v) \neq \Gamma$, it turns out that $O_\Gamma(v)$ is a circle. In this way we have \mathbb{T}/Γ split in one frequency sets $O_\Gamma(v)$. Consequently \mathbb{T}/Γ is also a circle, because \mathbb{T} is a 2-torus. The semiflow φ^t on \mathbb{T} is defined for all $t \geq 0$ provided that \mathbb{T} is bounded and invariant. Restricted to \mathbb{T} , φ^t induces a semiflow Ψ^t on \mathbb{T}/Γ given by $\Psi^t(O_\Gamma(w)) = O_\Gamma(\varphi^t(w))$, as can be checked easily.

Let S be the set of fixed points of Ψ^t . If $O_\Gamma(w) \in S$, then $O_\Gamma(\varphi^t(w)) = O_\Gamma(w)$ for all $t \geq 0$, what implies $O_\Gamma(w) = O_\varphi(w)$ and by a) of lemma A.9 $\varphi^t(w)$ is a rotating wave. In addition, if $S \neq \emptyset$ then $\Psi^t(O_\Gamma(w)) \rightarrow S$ as $t \rightarrow \infty$ for all w in \mathbb{T} , i.e. w is asymptotic to a rotating wave. Therefore from the hypothesis $S = \emptyset$ and since \mathbb{T}/Γ is a circle and Ψ^t a semiflow, there exists $T > 0$ such that $\Psi^T(O_\Gamma(w)) = O_\Gamma(w)$ for some $w \in \mathbb{T}$: $O_\Gamma(w)$ is a periodic solution for Ψ^t on \mathbb{T}/Γ . This means for instance that $\varphi^T(w) = R_\theta(w)$ for some $\theta \in \Gamma$, or equivalently $Z^+(w) \neq \Gamma(w)$. From lemma A.7 we know that $\varphi^t(w)$ has a unique extension w_t defined for all $t \in \mathbb{R}$. Thus Ψ^t is actually a flow, putting $\Psi^{-t}(O_\Gamma(w_s)) = O_\Gamma(w_{s-t})$. Moreover, every Γ -orbit on \mathbb{T} contains w_t for some t , seeing that $\Psi^t(O_\Gamma(w))$ traverses the whole circle \mathbb{T}/Γ . Hence if $v \in \mathbb{T}$, there exists t such that $w_t \in O_\Gamma(v)$. This implies $\varphi^t(w) = R_{\bar{\theta}}(v)$, for some $\bar{\theta} \in \Gamma$. On the other hand

$$\begin{aligned} \varphi^T(w) = R_\theta(w) &\implies \varphi^{t+T}(w) = \varphi^t(R_\theta(w)) \implies \varphi^T(\varphi^t(w)) = R_\theta(\varphi^t(w)) \\ &\implies \varphi^T(R_{\bar{\theta}}(v)) = R_\theta(R_{\bar{\theta}}(v)) \implies \varphi^T(v) = R_\theta(v), \end{aligned}$$

and from here $Z^+(v) \neq \Gamma(v)$, which together with $O_\Gamma(v) \neq O_\varphi(v)$ prove the result using b) of lemma A.9. \square

In the following we consider a modulated wave with modulation data (s, τ, Φ) and associated invariant torus \mathbb{T} . We also take m a fixed multiple of s , which represent the number of wave peaks the wave pattern has.

Definition A.15. A continuous function $\Theta : \mathbb{T} \rightarrow \mathbb{S}^1$ is a phase-function if $\Theta(R_\theta(v)) = e^{i\alpha m\theta} \Theta(v)$ for all $v \in \mathbb{T}$ and $\alpha = 2\pi/L$.

If v_t is a rotating wave with order of symmetry m , i.e. $\tilde{\Gamma}(v_t) = (L/m)\mathbb{Z}$, and $\gamma = \{v_t : t \geq 0\}$, then any function $\Theta : \gamma \rightarrow \mathbb{S}^1$ satisfies $\Theta(v) = \Theta(R_{L/m}(v))$, what justifies the inclusion of m in definition A.15, together with the need that measurements in the modulated régime are to correspond to those in any previous rotating wave régime.

Definition A.16. Given a phase function Θ and a solution $v_t = \varphi^t(v)$, $v \in \mathbb{T}$, let $\psi(t)$ a continuous function such that $\psi(0) = 0$ and $\exp(i\alpha\psi(t)) = \Theta(v_t)\Theta(v_0)^{-1}$. We define the phase velocity for Θ as $c_\Theta = \lim_{t \rightarrow \infty} \psi(t)/mt$.

Lemma A.17. The phase velocity is related to the modulation data by $c_\Theta = (\Phi - rL/m)/\tau$ for some $r \in \mathbb{Z}$. Furthermore c_Θ is independent on $v \in \mathbb{T}$.

Proof: From the modulation data, $\varphi^\tau(v) = R_\Phi(v_0)$ and then $\Theta(v_\tau) = e^{i\alpha m \Phi} \Theta(v_0)$. Hence $\psi(\tau) = m\Phi - rL$ for some $r \in \mathbb{Z}$. Analogously for $n \in \mathbb{Z}$

$$\begin{aligned} \exp(i\alpha\psi(n\tau + t)) &= \Theta(v_{n\tau+t})\Theta(v_0)^{-1} = \Theta(R_{n\Phi}(v_t))\Theta(v_0)^{-1} = e^{i\alpha mn\Phi} \Theta(v_t)\Theta(v_0)^{-1} \\ &= (\Theta(v_\tau)\Theta(v_0)^{-1})^n \Theta(v_t)\Theta(v_0)^{-1} = \exp(i\alpha(n\psi(\tau) + \psi(t))), \end{aligned}$$

which yields $\psi(n\tau + t) = n\psi(\tau) + \psi(t) + k(t)L$ for $k(t) \in \mathbb{Z}$. This relation for $n = 1$ gives $\psi(\tau + t) = \psi(\tau) + \psi(t) + k(t)L$ and due to the continuity of $\psi(t)$ and that $k(0) = 0$, we get $k(t) = 0$ for all t . In the general case, by induction on n , it also results $k(t) = 0$ for all t . The phase velocity is now readily obtained by

$$c_\Theta = \lim_{t \rightarrow \infty} \frac{\psi(t)}{mt} = \lim_{\substack{n \rightarrow \infty \\ 0 \leq t < \tau}} \frac{n\psi(\tau) + \psi(t)}{m(n\tau + t)} = \frac{\psi(\tau)}{m\tau} = \frac{\Phi}{\tau} - \frac{rL}{m\tau}.$$

In the proof of theorem A.14 it is shown that if $u, v \in \mathbb{T}$ then $w = R_\theta \varphi^{\bar{t}}(v)$ for some $\bar{t} \geq 0$ and some $\theta \in \Gamma$. As in definition A.16 we introduce a continuous function $\bar{\psi}(t)$ such that $\bar{\psi}(0) = 0$ and $\exp(i\alpha\bar{\psi}(t)) = \Theta(w_t)\Theta(w_0)^{-1}$. The relation with $\psi(t)$ is given by

$$\begin{aligned} \exp(i\alpha\bar{\psi}(t)) &= \Theta(w_t)\Theta(w_0)^{-1} = \Theta(\varphi^{\bar{t}} R_\theta(v_{\bar{t}}))\Theta(R_\theta(v_{\bar{t}}))^{-1} = \Theta(v_{\bar{t}+t})\Theta(v_{\bar{t}})^{-1} \\ &= \Theta(v_{\bar{t}+t})\Theta(v_0)^{-1} (\Theta(v_{\bar{t}})\Theta(v_0)^{-1})^{-1} = \exp[i\alpha(\psi(\bar{t} + t) - \psi(\bar{t}))], \end{aligned}$$

and so $\bar{\psi}(t) = \psi(\bar{t} + t) - \psi(\bar{t}) + k(t)L$ for $k(t) \in \mathbb{Z}$. Since $k(t)$ must be continuous and integer and $k(0) = 0$, then $k(t) = 0$ for all t . The phase velocity \bar{c}_Θ for $\bar{\psi}$ is

$$\bar{c}_\Theta = \lim_{t \rightarrow \infty} \frac{\bar{\psi}(t)}{mt} = \lim_{t \rightarrow \infty} \frac{\psi(\bar{t} + t) - \psi(\bar{t})}{mt} = \lim_{t \rightarrow \infty} \frac{\psi(\bar{t} + t)}{mt} = c_\Theta. \quad \square$$

Theorem A.18. For an observer in a frame of reference which translates in the stream direction with constant velocity c_Θ , the state of the system at time $t + \tau$ is the state at time t translated by nL/m , for $n \in \mathbb{Z}$ such that $n = r \bmod m/s$ and $0 \leq n < m/s$.

Proof: Let us choose $n \in \mathbb{Z}$ such that

$$\begin{aligned} n = r \bmod m/s, \quad 0 \leq n < m/s &\iff r = km/s + n, \quad k \in \mathbb{Z}, \quad 0 \leq n < m/s \\ &\iff rL/m = kL/s + nL/m, \quad k \in \mathbb{Z}, \quad 0 \leq nL/m < L/s. \end{aligned}$$

From the modulation data (s, τ, Φ) , $\Gamma(\mathbf{u}) = L/s\mathbb{Z}$, and therefore $R_{rL/m} = R_{nL/m}$. As in the comments following definition A.4, we consider a translation of θ in the stream direction x by $R_\theta(\mathbf{u}(x, y, t)) = \mathbf{u}(x - \theta, y, t)$. We denote as $\tilde{x} = x - c_\Theta t$, the position of x at time t viewed

by the observer and $\tilde{\mathbf{u}}(\tilde{x}, y, t)$ the state of the system in the moving frame of reference. The relationship between both systems of coordinates is given by $\tilde{\mathbf{u}}(\tilde{x}, y, t) = \mathbf{u}(\tilde{x} + c_{\Theta}t, y, t) = R_{-c_{\Theta}t}(\mathbf{u}(x, y, t))$, and hence at time τ , applying lemma A.17, we have

$$\begin{aligned}\tilde{\mathbf{u}}(\tilde{x}, y, \tau) &= R_{-c_{\Theta}\tau}(\mathbf{u}(x, y, \tau)) = R_{\Phi - c_{\Theta}\tau}(\mathbf{u}(x, y, 0)) \\ &= R_{\tau L/m}(\mathbf{u}(x, y, 0)) = R_{nL/m}(\mathbf{u}(x, y, 0)),\end{aligned}$$

and the proof is completed. □

B

Appendix

Interpolation

In this appendix we review some basic results on interpolation by means of periodic functions and Chebyshev polynomials.

B.1 Discrete Fourier series

We consider in this section some properties of Fourier series which are relevant to the application of Galerkin's spectral method (see § 2.1 and § 2.3). One of the main convergence properties of spectral methods are based upon the

Proposition B.1. *Let us suppose $u(x)$ an infinitely differentiable function in $[0, L]$ and L -periodic for which*

$$u(x) = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ik\alpha x}, \quad \hat{u}_k = \frac{1}{L} \int_0^L u(x) e^{-ik\alpha x} dx, \quad \alpha = \frac{2\pi}{L}.$$

Then $\hat{u}_k = O(k^{-m})$ for all $m \in \mathbb{N}$, i.e. \hat{u}_k decays faster than any negative power of k . If in addition $u(x)$ is analytic, then $\hat{u}_k = O(\exp(-c|k|))$ for some positive constant c .

Proof: Integrating by parts we have

$$\begin{aligned} L\hat{u}_k &= \int_0^L u(x) e^{-ik\alpha x} dx = \frac{-1}{ik\alpha} (u(L^-) - u(0^+)) + \frac{-1}{ik\alpha} \int_0^L u'(x) e^{-ik\alpha x} dx \\ &= \frac{-1}{ik\alpha} \int_0^L u'(x) e^{-ik\alpha x} dx. \end{aligned}$$

This proves that $\hat{u}_k = O(k^{-1})$. Applying the same process m times to the last integral, we conclude that $\hat{u}_k = O(k^{-m})$ for all $m \in \mathbb{N}$.

We suppose first that $k < 0$. If $u(x)$ is analytic in \mathbb{R} then it is also analytic as a complex function in the rectangle $\mathcal{R} = [0, L] \times [0, \rho]$, for $\rho > 0$. Let $\Gamma = \partial\mathcal{R}$ be the positively oriented boundary of

\mathcal{R} and put $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$, such that $\Gamma_1 = \{x, x \in [0, L]\}$, $\Gamma_3 = \{x + \rho i, x \in [0, L]\}$, $\Gamma_2 = \{L + yi, y \in [0, \rho]\}$ and $\Gamma_4 = \{yi, y \in [0, \rho]\}$. If $f(x + L + yi) = f(x + yi)$ for $x, y \in \mathbb{R}$, it turns out that

$$\begin{aligned} \int_{\Gamma_2} f(z) dz &= \int_0^\rho f(L + ti)i dt = i \int_0^\rho f(ti) dt \\ &= -i \int_0^\rho f((1-s)i) ds = - \int_{\Gamma_4} f(z) dz. \end{aligned}$$

By the theory of analytic functions we know that $\int_\gamma f = 0$ if γ is a path homotopic to a point and f analytic on an open set A such that $\gamma \subset A$. We can apply this result to our situation for $\gamma = \Gamma$, $f(z) = u(z)e^{ik\alpha z}$ and $f(x + L + yi) = f(x + yi)$, and we have

$$\begin{aligned} 0 &= \int_\Gamma u(z)e^{ik\alpha z} dz = \left(\int_{\Gamma_1} + \int_{\Gamma_2} + \int_{\Gamma_3} + \int_{\Gamma_4} \right) u(z)e^{ik\alpha z} dz \\ &= \left(\int_{\Gamma_1} + \int_{\Gamma_3} \right) u(z)e^{ik\alpha z} dz = \int_0^L u(x)e^{ik\alpha x} dx + \int_{\Gamma_3} u(z)e^{ik\alpha z} dz. \end{aligned}$$

Therefore

$$\begin{aligned} |\hat{u}_k| &= \frac{1}{L} \left| \int_0^L u(x)e^{-ik\alpha x} dx \right| = \frac{1}{L} \left| \int_{\Gamma_1} u(z)e^{-ik\alpha z} dz \right| \\ &= \frac{1}{L} \left| \int_{\Gamma_3} u(z)e^{-ik\alpha z} dz \right| = \frac{1}{L} \left| \int_0^L u(x + \rho i)e^{-ik\alpha(x + \rho i)} dx \right| \\ &\leq \frac{1}{L} \int_0^L |u(x + \rho i)e^{-ik\alpha(x + \rho i)}| dx \leq \frac{A}{L} \int_0^L e^{k\alpha\rho} dx = Ae^{k\alpha\rho}, \end{aligned}$$

being A an upper bound of $u(x + \rho i)$ for $x \in [0, L]$. If $k \geq 0$ the result follows the same lines taking $\mathcal{R} = [0, L] \times [\rho, 0]$ for $\rho < 0$. \square

Now we state a result about polynomial interpolation by trigonometric functions, which is used for instance in the evaluation of convolution sums (2.14).

Proposition B.2. *Given $2N + 1$ complex values w_0, \dots, w_{2N} of certain function $w(x)$ at the abscissae $x_j = jL/(2N + 1)$, for $j = 0, \dots, 2N$ We construct*

$$p(x) \stackrel{\text{def}}{=} \sum_{k=-N}^N \tilde{w}_k e^{ik\alpha x}, \quad \tilde{w}_k \stackrel{\text{def}}{=} \frac{1}{2N + 1} \sum_{j=0}^{2N} w_j e^{-ik\alpha x_j} \quad (\text{B.1})$$

Then the coefficients \tilde{w}_k are the only ones such that $p(x)$ interpolates $w(x)$, i.e. $p(x_j) = w_j$ for $j = 0, \dots, 2N$.

Proof: Let us verify that $p(x_j) = w_j$ if and only if \tilde{w}_k are as defined in (B.1) and this will prove existence and uniqueness of $p(x)$. We define z, z_j and $z^{(k)}$ by

$$\begin{aligned} z &= e^{i\alpha x}, \quad z_j = e^{i\alpha x_j}, \quad j = 0, \dots, 2N, \\ z^{(k)} &= (1, z_1^k, \dots, z_{2N}^k) \in \mathbb{C}^{2N+1}, \quad k = 0, \dots, 2N. \end{aligned}$$

From the standard scalar product in \mathbb{C}^{2N+1} we have for $k, l = 0, \dots, 2N$ and $p = k - l$, the orthogonality relation

$$\begin{aligned} \langle z^{(k)}, z^{(l)} \rangle &= \sum_{j=0}^{2N} z_j^k z_j^{-l} = \sum_{j=0}^{2N} e^{ip\alpha x_j} = \sum_{j=0}^{2N} \left(e^{ip \frac{2\pi}{2N+1}} \right)^j \\ &= \begin{cases} 2N+1, & \text{if } p = m(2N+1), m \in \mathbb{Z} \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \quad (\text{B.2})$$

If we put $W = (w_0, \dots, w_{2N})^t$ then

$$w_j = p(x_j) = \sum_{k=-N}^N \tilde{w}_k e^{ik\alpha x_j} = \sum_{k=0}^{2N} \tilde{w}_k z_k^j, \quad j = 0, \dots, 2N,$$

is equivalent to

$$W = \tilde{w}_0 z^{(0)} + \dots + \tilde{w}_{2N} z^{(2N)}.$$

Therefore from (B.2)

$$\begin{aligned} \frac{1}{2N+1} \sum_{j=0}^{2N} w_j e^{-ik\alpha x_j} &= \frac{1}{2N+1} \sum_{j=0}^{2N} w_j z_j^{-k} = \frac{1}{2N+1} \langle W, z^{(k)} \rangle \\ &= \frac{1}{2N+1} \langle \tilde{w}_0 z^{(0)} + \dots + \tilde{w}_{2N} z^{(2N)}, z^{(k)} \rangle = \tilde{w}_k. \quad \square \end{aligned}$$

The finite series in (B.1) define the inverse and direct discrete Fourier transforms of a set of complex values $\tilde{w}_{-N}, \dots, \tilde{w}_N$ and w_0, \dots, w_{2N} respectively. To compute those transforms we make use of fast Fourier transforms (FFT). We now show an application of FFT to compute cosine transforms.

Proposition B.3. *Supposing M even for simplicity and given real numbers w_0, \dots, w_M , the values $\tilde{w}_0, \dots, \tilde{w}_M$ of the cosine transform C_1 defined in (2.7), can be extracted by applying a discrete Fourier transform to y_m*

$$y_m \stackrel{\text{def}}{=} \frac{1}{2}(w_m + w_{M-m}) - \sin \frac{\pi m}{M}(w_m - w_{M-m}), \quad m = 0, \dots, M-1.$$

More precisely, if we put as in (B.1)

$$\tilde{y}_j = R_j + iI_j = \frac{1}{M} \sum_{m=0}^{M-1} y_m e^{-2\pi i j m / M}, \quad j = 0, \dots, \frac{M}{2},$$

then we have the recurrence

$$\begin{aligned} \tilde{w}_1 &= \frac{2}{M} \sum_{m=0}^M \frac{w_m}{\bar{c}_m} \cos \frac{\pi m}{M}, \\ \bar{c}_{2j+1} \tilde{w}_{2j+1} &= \bar{c}_{2j-1} \tilde{w}_{2j-1} - 2I_j, & j &= 1, \dots, M/2 - 1, \\ \tilde{w}_{2j} &= 2/\bar{c}_{2j} R_j, & j &= 0, \dots, M/2, \end{aligned}$$

where $\bar{c}_0 = \bar{c}_M = 2$, $\bar{c}_j = 1$ if $j \neq 0, M$. Conversely, if we reverse this algorithm, from starting values $\tilde{w}_0, \dots, \tilde{w}_M$, we recover w_0, \dots, w_M , i.e. the inverse cosine transform.

Proof: The recurrence follows at once from the following formulas for $j = 0, \dots, M/2$

$$\begin{aligned}
MI_j &= - \sum_{m=0}^{M-1} y_m \sin \frac{2\pi jm}{M} \\
&= - \sum_{m=1}^{M-1} \left[\frac{1}{2}(w_m + w_{M-m}) - \sin \frac{\pi m}{M}(w_m - w_{M-m}) \right] \sin \frac{2\pi jm}{M} \\
&= - \sum_{m=1}^{M-1} \frac{w_m}{2} \sin \frac{2\pi jm}{M} + \sum_{m=1}^{M-1} \frac{w_m}{2} \sin \frac{2\pi jm}{M} \\
&\quad + \sum_{m=1}^{M-1} w_m \sin \frac{\pi m}{M} \sin \frac{2\pi jm}{M} + \sum_{m=1}^{M-1} w_m \sin \frac{\pi m}{M} \sin \frac{2\pi jm}{M} \\
&= 2 \sum_{m=1}^{M-1} w_m \sin \frac{\pi m}{M} \sin \frac{2\pi jm}{M} \\
&= \sum_{m=1}^{M-1} w_m \left(\cos \frac{\pi m}{M}(2j-1) - \cos \frac{\pi m}{M}(2j+1) \right) \\
&= \frac{M\bar{c}_{2j-1}}{2} \tilde{w}_{2j-1} - \frac{M\bar{c}_{2j+1}}{2} \tilde{w}_{2j+1}, \\
MR_j &= \sum_{m=0}^{M-1} y_m \cos \frac{2\pi jm}{M} \\
&= \sum_{m=0}^{M-1} \left[\frac{1}{2}(w_m + w_{M-m}) - \sin \frac{\pi m}{M}(w_m - w_{M-m}) \right] \cos \frac{2\pi jm}{M} \\
&= \sum_{m=0}^{M-1} \frac{w_m}{2} \cos \frac{2\pi jm}{M} + \sum_{m=1}^M \frac{w_m}{2} \cos \frac{2\pi jm}{M} \\
&\quad + \sum_{m=1}^M w_m \sin \frac{\pi m}{M} \cos \frac{2\pi jm}{M} - \sum_{m=0}^{M-1} w_m \sin \frac{\pi m}{M} \cos \frac{2\pi jm}{M} \\
&= \sum_{m=0}^M \frac{w_m}{\bar{c}_m} \cos \frac{2\pi jm}{M} = \frac{M\bar{c}_{2j}}{2} \tilde{w}_{2j}.
\end{aligned}$$

In order to reverse the algorithm, we first utilize the recurrence to find \tilde{y}_j for $j = 0, \dots, M/2$. By means of an inverse discrete Fourier transform we deduce y_0, \dots, y_{M-1} , and from the definition of y_m we get the relations

$$\begin{aligned}
y_m + y_{M-m} &= w_m + w_{M-m}, \\
y_m - y_{M-m} &= -2 \sin(\pi m/M)(w_m + w_{M-m}),
\end{aligned}$$

which combined for $m = 0, \dots, M$ finally give

$$w_m = \frac{1}{2}(y_m + y_{M-m}) - \frac{y_m - y_{M-m}}{4 \sin(\pi m/M)}. \quad \square$$

From this proposition and recurrence (2.9) we have an efficient algorithm to calculate y -derivatives of u and v on the first grid y_m defined in (2.4).

B.2 Basic results on orthogonal polynomials

The results in this section are connected with §2.2. We show the importance of Chebyshev abscissae as collocation points in spectral methods. Let us first consider basic facts about Gaussian quadratures and orthogonal polynomials. On the linear space $L_\omega^2[a, b]$ of functions for which $\int_a^b (f(x))^2 \omega(x) dx$ is finite, we define the scalar product

$$\langle f, g \rangle \stackrel{\text{def}}{=} \int_a^b f(x)g(x)\omega(x) dx, \quad (\text{B.3})$$

where $\omega(x)$ is a positive continuous function on (a, b) . The associated norm is defined by $\|f\|^2 = \langle f, f \rangle$. Let \mathcal{P}_n the set of polynomials of degree n or less. The following three results are proved on almost any book on numerical methods (see for instance Johnson & Riess 1977).

Theorem B.4. *For the scalar product (B.3) there exists a family of monic orthogonal polynomials $p_n(x)$ for $n = 0, 1, 2, \dots$, such that $p_n \in \mathcal{P}_n$ and satisfy the recurrence*

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_n(x) = (x - a_n)p_{n-1}(x) - b_n p_{n-2}(x), \quad n \geq 2, \quad (\text{B.4})$$

where $a_n = \langle x p_{n-1}, p_{n-1} \rangle / \langle p_{n-1}, p_{n-1} \rangle$ and $b_n = \langle p_{n-1}, p_{n-1} \rangle / \langle p_{n-2}, p_{n-2} \rangle$. Besides p_n has n real distinct roots in (a, b) .

Theorem B.5. *The quadrature formula $\int_a^b p(x)\omega(x) dx = \sum_{l=0}^n r_l p(x_l)$ holds for all $p \in \mathcal{P}_{2n+1}$ if and only if $\{x_l\}_{l=0}^n$ are the zeros of p_{n+1} and $r_l = \langle L_l, 1 \rangle$ for $l = 0, \dots, n$, where $L_l \in \mathcal{P}_n$ is such that $L_l(x_k) = \delta_{lk}$.*

Theorem B.6. *Let $f \in L_\omega^2[a, b]$, then the polynomial $p_n^* \in \mathcal{P}_n$ which satisfies $\|f - p_n^*\| \leq \|f - p\|$ for all $p \in \mathcal{P}_n$ is given by*

$$p_n^*(x) = \sum_{j=0}^n \langle f, \bar{p}_j \rangle \bar{p}_j(x),$$

where $\bar{p}_j = p_j / \|p_j\|$, are orthonormal polynomials. In addition $\lim_{n \rightarrow \infty} \|f - p_n^*\| = 0$, that is to say, p_n^* converges to f in $L_\omega^2[a, b]$.

When $[a, b] = [-1, 1]$ and $\omega(y) = (1 - y^2)^{-1/2}$ then the Chebyshev polynomials $T_m(y) = \cos(m \arccos(y))$ for $m = 0, 1, 2, \dots$ are a family of non-monic orthogonal polynomials. The trigonometric relation $\cos(m+1)\theta + \cos(m-1)\theta = 2 \cos \theta \cos m\theta$ gives rise to the recurrence

$$T_0(y) = 1, \quad T_1(y) = y, \quad T_{m+1}(y) = 2yT_m(y) - T_{m-1}(y), \quad m = 1, 2, \dots$$

Moreover, it is easily check that $\langle T_0, T_0 \rangle = \pi$, $\langle T_m, T_m \rangle = \pi/2$, for $m \geq 1$, $\langle T_m, T_n \rangle = 0$ for $m \neq n$. The rapid convergence of Chebyshev expansions is a direct consequence of proposition B.1.

Proposition B.7. Let $f(y)$ be an infinitely differentiable function in $[-1, 1]$, such that it can be expanded in Chebyshev series (cf. theorem B.6)

$$f(y) = \sum_{k=0}^{\infty} \hat{f}_k T_k(y), \quad \hat{f}_k = \frac{\langle f, T_k \rangle}{\langle T_k, T_k \rangle} = \frac{2}{\pi c_k} \int_{-1}^1 \frac{f(y) T_k(y)}{\sqrt{1-y^2}} dy, \quad (\text{B.5})$$

where $c_0 = 2$ and $c_k = 1$ for $k \geq 2$. Then $\hat{f}_k = O(k^{-m})$ for every $m \in \mathbb{N}$. If in addition $u(x)$ is analytic, then $\hat{f}_k = O(\exp(-c|k|))$ for some positive constant c .

Proof: By means of the change $x = \cos \theta$, we define

$$\bar{f}(\theta) \stackrel{\text{def}}{=} f(\cos \theta) = \sum_{k=0}^{\infty} \hat{f}_k T_k(\cos \theta) = \sum_{k=0}^{\infty} \hat{f}_k \cos(k\theta).$$

For this is a particular case of a Fourier series, applying proposition B.1 we obtain the result. \square

Once the interesting convergence property of Chebyshev expansions (B.5) is shown, we focus on the truncated series up to order say M and how to approximate the Chebyshev coefficients $\langle f, T_k \rangle$. Because such coefficients are defined by an integral, this will be accomplished by Gauss quadrature formulas as in theorem B.5. To that end we need to know the roots x_l of the orthogonal polynomials and the weights r_l . For the case of Chebyshev polynomials the roots are straightforward to find as

$$T_M(\bar{y}_m) = 0 \iff \bar{y}_m = \cos \frac{\pi(2m+1)}{2M}, \quad m = 0, \dots, M-1. \quad (\text{B.6})$$

To compute the weights r_l we need the

Theorem B.8. *Introducing the sequence of polynomials*

$$\begin{aligned} \phi_0(x) &= 0, & \phi_1(x) &= \int_a^b \omega(t) dt, \\ \phi_k(x) &= (x - a_k)\phi_{k-1}(x) - b_k\phi_{k-2}(x), & \text{for } k &\geq 2, \end{aligned}$$

and a_k and b_k as defined in (B.4), then one has $\eta = \phi_{n+1}(x_l)/p'_{n+1}(x_l)$, for $l = 0, \dots, n$.

Proof: Let first check by induction that

$$\phi_n(x) = \int_a^b \frac{p_n(t) - p_n(x)}{t-x} \omega(t) dt. \quad (\text{B.7})$$

This is evidently true for $n = 0, 1$. Assume (B.7) is valid for $k < n$. From (B.4)

$$\begin{aligned} \phi_n(x) &= (x - a_n)\phi_{n-1}(x) - b_n\phi_{n-2}(x) \\ &= \int_a^b \left[(x - a_n) \frac{p_{n-1}(t) - p_{n-1}(x)}{t-x} - b_n \frac{p_{n-2}(t) - p_{n-2}(x)}{t-x} \right] \omega(t) dt \\ &= \int_a^b \frac{(t - a_n)p_{n-1}(t) - p_{n-2}(t) - (x - a_n)p_{n-1}(x) - p_{n-2}(x)}{t-x} \omega(t) dt \\ &= \int_a^b \frac{p_n(t) - p_n(x)}{t-x} \omega(t) dt. \end{aligned}$$

Now $L_l(x) = p_{n+1}(x)/[(x - x_l)p'_{n+1}(x_l)]$ for $l = 0, \dots, n$, as it is easily verified, and then

$$\frac{\phi_{n+1}(x_l)}{p'_{n+1}(x_l)} = \int_a^b \frac{p_{n+1}(t) - p_{n+1}(x_l)}{(t - x_l)p'_{n+1}(x_l)} \omega(t) dt = \int_a^b L_l(t) \omega(t) dt = r_l. \quad \square$$

Let us return to the computation of the weights r_l for the case of Chebyshev polynomials. The associated monic orthogonal polynomials are simply

$$p_0(y) = 1, \quad p_m(y) = 2^{1-m} T_m(y), \quad m \geq 1,$$

which in view of the recurrence of Chebyshev polynomials drives to

$$p_0(y) = 1, \quad p_1(y) = y, \quad p_m(y) = yp_{m-1}(y) - b_m p_{m-2}(y), \quad m \geq 2,$$

being $b_2 = 1/2$ and $b_m = 1/4$ for $m > 2$. As a result the recurrence for ϕ_k is

$$\begin{aligned} \phi_0(y) &= 0, & \phi_1(y) &= \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \langle T_0, T_0 \rangle = \pi, \\ \phi_m(y) &= yp_{m-1}(y) - b_m \phi_{m-2}(y), \quad m \geq 2. \end{aligned}$$

We need to introduce the second kind Chebyshev polynomials $Q_m(y) = T'_{m+1}(y)/(m+1) = \sin((m+1)\theta)/\sin(\theta)$ for $\theta = \arccos(y)$, which in view of the identity $\sin((m+2)\theta) + \sin(m\theta) = 2 \cos \theta \sin((m+1)\theta)$, satisfy the recurrence $Q_0(y) = 1$, $Q_1(y) = 2y$, $Q_m(y) = 2yQ_{m-1}(y) - Q_{m-2}(y)$ for $m \geq 2$. Thus, defining $q_m(y) = 2^{-m} Q_m(y)$ we obtain $q_0(y) = 1$, $q_1(y) = y$, $q_m(y) = yq_{m-1}(y) - q_{m-2}(y)/4$ for $m \geq 2$, a recurrence very similar to the one for ϕ_m . In particular $\phi_2 = \pi y = \pi q_1$, $\phi_3 = \pi(y^2 - 1/4) = \pi q_2$, and since the recurrence for ϕ_m and q_m coincides for $m \geq 3$ we conclude that $\phi_m = \pi q_{m-1}$ for $m \geq 1$. Finally we can derive, according to theorem B.8, the expression of r_l associated with \bar{y}_m , defined in (B.6), by

$$r_l = \frac{\phi_M(\bar{y}_l)}{p'_M(\bar{y}_l)} = \frac{\pi 2^{1-M} Q_{M-1}(\bar{y}_l)}{M 2^{1-M} Q_{M-1}(\bar{y}_l)} = \frac{\pi}{M}, \quad l = 0, \dots, M-1.$$

The quadrature formula is expressed as

$$\int_{-1}^1 \frac{p(y)}{\sqrt{1-y^2}} dy \approx \frac{\pi}{M} \sum_{m=0}^{M-1} p(\bar{y}_m), \quad (\text{B.8})$$

which is exact for $p \in \mathcal{P}_{2M-1}$. Quadrature formula of theorem B.5 allows us to introduce a discrete scalar product for any two functions f, g defined in $[a, b]$ by

$$\langle f, g \rangle_d \stackrel{\text{def}}{=} \sum_{l=0}^n r_l f(x_l) g(x_l),$$

and from here the result on interpolating polynomials.

Theorem B.9. Let $\{x_l\}_{l=0}^n$ be the zeros of p_{n+1} (as in theorem B.5), and $P(x) = \sum_{k=0}^n s_k p_k(x)$. The condition $s_k = \langle p_m, f \rangle_d / \langle p_m, p_m \rangle_d$ for $k = 0, \dots, n$, is equivalent to $P(x_l) = f(x_l)$ for $l = 0, \dots, n$.

Proof: As it is well known the interpolating polynomial exists and is unique and thus can be written in the form $P(x) = \sum_{k=0}^n s_k p_k(x)$. If for $l = 0, \dots, n$, $P(x_l) = f(x_l)$, then

$$\begin{aligned} \langle p_m, f \rangle_d &= \sum_{l=0}^n r_l p_m(x_l) f(x_l) = \sum_{l=0}^n r_l p_m(x_l) \sum_{k=0}^n s_k p_k(x_l) \\ &= \sum_{k=0}^n s_k \sum_{l=0}^n r_l p_m(x_l) p_k(x_l) = \sum_{k=0}^n s_k \langle p_m, p_k \rangle_d = s_m \langle p_m, p_m \rangle_d. \end{aligned}$$

The last equality is a consequence of the orthogonality of p_k for the continuous scalar product and $\langle p_k, p_m \rangle_d = \langle p_k, p_m \rangle$, if $p_k p_m \in \mathcal{P}_{2n+1}$, which is another statement of the quadrature formula in theorem B.5. \square

Another interpretation of this theorem is that, if for expansion (B.5) we truncate it up to order $M - 1$ and approximate \hat{f}_k for $k = 0, \dots, M - 1$ by means of (B.8), we find that

$$\begin{aligned} \hat{f}_k &= \frac{\langle f, T_k \rangle}{\langle T_k, T_k \rangle} = \frac{2}{\pi c_k} \int_{-1}^1 \frac{f(y) T_k(y)}{\sqrt{1-y^2}} dy \approx \frac{2}{M c_k} \sum_{m=0}^{M-1} f(\bar{y}_m) T_k(\bar{y}_m) \\ &= \frac{\langle f, T_k \rangle_d}{\langle T_k, T_k \rangle_d} = \frac{2}{M c_k} \sum_{m=0}^{M-1} f(\bar{y}_m) \cos \frac{\pi(2m+1)k}{2M} \stackrel{\text{def}}{=} \tilde{f}_k, \end{aligned} \quad (\text{B.9})$$

and so the approximating series is precisely the interpolating polynomial of theorem B.9. We derive the relation between \hat{f}_k and \tilde{f}_k by

$$\begin{aligned} \tilde{f}_k &= \frac{2}{M c_k} \sum_{m=0}^{M-1} f(\bar{y}_m) T_k(\bar{y}_m) = \frac{2}{M c_k} \sum_{m=0}^{M-1} \left(\sum_{j=0}^{\infty} \hat{f}_j T_j(\bar{y}_m) \right) T_k(\bar{y}_m) \\ &= \frac{2}{M c_k} \sum_{j=0}^{\infty} \hat{f}_j \sum_{m=0}^{M-1} T_j(\bar{y}_m) T_k(\bar{y}_m) = \frac{2}{\pi c_k} \sum_{j=0}^{\infty} \hat{f}_j \langle T_j, T_k \rangle_d \\ &= \hat{f}_k - (\hat{f}_{2M-k} + \hat{f}_{2M+k}) + (\hat{f}_{4M-k} + \hat{f}_{4M+k}) - \dots \end{aligned}$$

The reason for the last step is that $T_{2M \pm l}(\bar{y}_m) = (-1)^p T_{|l|}(\bar{y}_m)$ and hence $\langle T_{|l|}, T_k \rangle_d = (-1)^p \langle T_{2M \pm l}, T_k \rangle_d$. As a consequence the error $|\hat{f}_k - \tilde{f}_k|$ decrease with the Fourier coefficients \hat{f}_j .

As we have seen, the Chebyshev abscissae $\bar{y}_m \in (-1, 1)$ for $m = 0, \dots, M - 1$, are important points for interpolating a function, but for some cases it is important to include also -1 and 1 among those points. Consider y_m the zeros of T'_M together with -1 and 1 , i.e. $y_m = \cos(\pi m/M)$ for $m = 0, \dots, M$. Given two functions f and g in $[-1, 1]$, we define another discrete scalar product

$$\langle f, g \rangle_{d'} \stackrel{\text{def}}{=} \sum_{m=0}^M \frac{f(y_m) g(y_m)}{\bar{c}_m}, \quad (\text{B.10})$$

where $\bar{c}_0 = \bar{c}_M = 2$, and $\bar{c}_m = 1$ for $m = 1, \dots, M - 1$. To prove that T_m are orthogonal polynomials for this scalar product we need the

Lemma B.10. Let $S_1(x) = \sum_{j=1}^M \cos jx$ and $S_2(x) = \sum_{j=0}^M \cos jx/\bar{c}_j$. Then

$$S_1(x) = \frac{1}{2} \left(\frac{\sin(M + 1/2)x}{\sin x/2} - 1 \right), \quad S_2(x) = \frac{\sin Mx \cos x/2}{2 \sin x/2}.$$

Proof: If $x = 2k\pi$ for $k \in \mathbb{Z}$ we can verify the formulae by L'Hôpital's rule. For $x \neq 2k\pi$, using the identity $2 \sin x/2 \cos jx = \sin(j + 1/2)x - \sin(j - 1/2)x$, yields

$$\begin{aligned} S_1(x) &= \sum_{j=1}^M \cos jx = \frac{1}{2 \sin x/2} \sum_{j=1}^M (\sin(j + 1/2)x - \sin(j - 1/2)x) \\ &= \frac{\sin(M + 1/2)x - \sin x/2}{2 \sin x/2} \\ S_2(x) &= \sum_{j=0}^M \frac{\cos jx}{\bar{c}_j} = \frac{1}{2} + S_1(x) - \frac{\cos Mx}{2} \\ &= \frac{\sin(M + 1/2)x - \cos Mx \sin x/2}{2 \sin x/2} = \frac{\sin Mx \cos x/2}{2 \sin x/2}. \end{aligned}$$

□

Theorem B.11. For the scalar product (B.10), and $0 \leq k, m \leq M$ it is satisfied

$$\langle T_k, T_m \rangle_{d'} = \frac{M}{2} \begin{cases} 0, & k \neq m \\ 1, & k = m, \quad 1 \leq k \leq M - 1 \\ 2, & k = m, \quad k = 0, M. \end{cases}$$

Proof: According to the lemma, for $0 \leq k \leq m \leq M$ we have,

$$\begin{aligned} \langle T_k, T_m \rangle_{d'} &= \sum_{j=0}^M \frac{T_k(y_j) T_m(y_j)}{\bar{c}_j} = \sum_{j=0}^M \frac{1}{\bar{c}_j} \cos \frac{\pi k j}{M} \cos \frac{\pi m j}{M} \\ &= \frac{1}{2} \sum_{j=0}^M \frac{1}{\bar{c}_j} \left(\cos \frac{\pi(m+k)j}{M} + \cos \frac{\pi(m-k)j}{M} \right) \\ &= \frac{\sin \pi(m+k) \cos \frac{\pi(m+k)}{2M}}{4 \sin \frac{\pi(m+k)}{2M}} + \frac{\sin \pi(m-k) \cos \frac{\pi(m-k)}{2M}}{4 \sin \frac{\pi(m-k)}{2M}}. \end{aligned}$$

If $m \neq k$ then both terms in the last expression vanishes, because the numerator is null and the denominator is not null. Conversely if $k = m$ evaluating S_2 directly, we obtain the announced result. □

We are in a position to formulate the interpolation result for the new abscisae y_m and a quadrature property, analogous to theorems B.9 and B.5 respectively.

Theorem B.12. Let $P(y) = \sum_{j=0}^M s_j T_j(y)$. The condition $s_j = \langle T_j, f \rangle_{d'} / \langle T_j, T_j \rangle_{d'}$ for $j = 0, \dots, M$, is equivalent to $P(y_m) = f(y_m)$ for $m = 0, \dots, M$.

Proof: We may express the unique interpolating polynomial as $P(y) = \sum_{j=0}^M s_j p_j(y)$. Because the orthogonality relations of theorem B.11 and imposing $P(y_m) = f(y_m)$ for $m = 0, \dots, M$, we have

$$\begin{aligned} \langle T_j, f \rangle_{d'} &= \sum_{m=0}^M \frac{T_j(y_m) f(y_m)}{\bar{c}_m} = \sum_{m=0}^M \frac{T_j(y_m)}{\bar{c}_m} \sum_{l=0}^M s_l T_l(y_m) \\ &= \sum_{l=0}^M s_l \sum_{m=0}^M \frac{T_j(y_m) T_l(y_m)}{\bar{c}_m} = \sum_{l=0}^M s_l \langle T_j, T_l \rangle_{d'} = s_j \langle T_j, T_j \rangle_{d'}. \quad \square \end{aligned}$$

Theorem B.13. The quadrature formula

$$\int_{-1}^1 \frac{f(y)}{\sqrt{1-y^2}} dy = \frac{\pi}{M} \sum_{m=0}^M \frac{f(y_m)}{\bar{c}_m}, \quad (\text{B.11})$$

is exact for $p \in \mathcal{P}_{2M-1}$ but not for $p \in \mathcal{P}_{2M}$.

Proof: We compare both formulae by means of respective scalar products, since

$$\langle T_0, f \rangle = \int_{-1}^1 \frac{f(y)}{\sqrt{1-y^2}} dy, \quad \langle T_0, f \rangle_{d'} = \sum_{m=0}^M \frac{f(y_m)}{\bar{c}_m}.$$

Truly from theorem B.11 and the orthogonality relations of Chebyshev polynomials, $\pi = \langle T_0, T_0 \rangle = \pi/M \langle T_0, T_0 \rangle_{d'}$, and $0 = \langle T_0, T_j \rangle$ for $j \geq 1$. On the other hand $\langle T_0, T_j \rangle_{d'} = 0$, for $j = 1, \dots, M$. Furthermore, because $T_{M+j}(y_m) = T_M(y_m) T_j(y_m)$ then $\langle T_0, T_{M+j} \rangle_{d'} = \langle T_M, T_j \rangle_{d'} = 0$, for $j = 1, \dots, M-1$ and the formula is exact up to order $2M-1$. However $\langle T_0, T_{2M} \rangle_{d'} = \langle T_M, T_M \rangle_{d'} = M$ and as a result the formula is not exact for every $p \in \mathcal{P}_{2M}$. \square

The quadrature formula (B.11) is not as in theorem B.5, as that would imply (B.11) to be of order $2M+1$. In spite of this we find similar properties. Considering again expansion (B.5), truncated up to order M and approximating \hat{f}_k for $k = 0, \dots, M$ by means of (B.11) we find that

$$\hat{f}_k = \frac{\langle f, T_k \rangle}{\langle T_k, T_k \rangle} \approx \tilde{f}_k \stackrel{\text{def}}{=} \frac{\langle f, T_k \rangle_{d'}}{\langle T_k, T_k \rangle_{d'}} = \frac{2}{M \bar{c}_k} \sum_{m=0}^M \frac{f(y_m)}{\bar{c}_m} \cos \frac{\pi k m}{M}, \quad (\text{B.12})$$

and so the approximating series is precisely the interpolating polynomial of theorem B.12. We derive the relation between \hat{f}_k and \tilde{f}_k by

$$\begin{aligned} \tilde{f}_k &= \frac{2}{M \bar{c}_k} \sum_{m=0}^M f(y_m) \frac{T_k(y_m)}{\bar{c}_m} = \frac{2}{M \bar{c}_k} \sum_{m=0}^M \left(\sum_{j=0}^{\infty} \hat{f}_j T_j(y_m) \right) \frac{T_k(y_m)}{\bar{c}_m} \\ &= \frac{2}{M \bar{c}_k} \sum_{j=0}^{\infty} \hat{f}_j \sum_{m=0}^M \frac{T_j(y_m) T_k(y_m)}{\bar{c}_m} = \frac{2}{M \bar{c}_k} \sum_{j=0}^{\infty} \hat{f}_j \langle T_j, T_k \rangle_{d'} \\ &= \hat{f}_k + (\hat{f}_{2M-k} + \hat{f}_{2M+k}) + (\hat{f}_{4M-k} + \hat{f}_{4M+k}) + \dots \end{aligned}$$

The reason for the last step is that $T_{2Mp \pm l}(y_m) = T_{|l|}(y_m)$ and so $\langle T_{|l|}, T_k \rangle_{d'} = \langle T_{2Mp \pm l}, T_k \rangle_{d'}$. From this relation we observe that the error $|\hat{f}_k - \tilde{f}_k|$ decrease with the Fourier coefficients \hat{f}_j .

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