Let $\Delta(\lambda) := \det W(\lambda)$. Then by the definition of $W(\lambda)$, Δ is an exponential polynomial [9] in λ. That is,

$$\Delta(\lambda) = \sum_{k=1}^{n} a_k \lambda^k e^{b_k \lambda},$$

where $a_k, b_k \in \mathbb{C}$ for $k \in \{1, \dots, n\}$.

Let X^{lj} be the $(n-1) \times (n-1)$ submatrix of the block matrix $\mathbb{W} := \begin{bmatrix} W & W \\ W & W \end{bmatrix}$, where X^{lj}_{11} is $\mathbb{W}_{l+1,j+1}$.

For $\lambda \in \mathbb{C}$ such that $\Delta(\lambda) \neq 0$, define

$$F^+_\lambda(f) := \frac{1}{2\pi\Delta(\lambda)} \sum_{l=1}^{n} \sum_{j=1} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) M^+_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx \tag{3.3a}$$

$$F^-_\lambda(f) := \frac{-e^{-i\lambda}}{2\pi\Delta(\lambda)} \sum_{l=1}^{n} \sum_{j=1} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) M^-_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\, dx. \tag{3.3b}$$

By the theory of exponential polynomials [9], the infimum of the distances between every two distinct zeroes of $\Delta(\lambda)$ is positive. Let 5ϵ be such this infimum. Let ∂S denote boundary of set S. Let $\operatorname{cl} S$ denote the closure of set S. Let $\mathbb{C}^\pm$ denote the open upper and open lower halves of the complex plane, respectively. Let $D(x_0, \epsilon)$ denote the disk $\{x \in \mathbb{C} : |x - x_0| < \epsilon\}$ centered at x_0 with radius ϵ. Let $C(x_0, \epsilon)$ denote the circle $\{x \in \mathbb{C} : |x - x_0| = \epsilon\}$ centered at x_0 with radius ϵ. Define the contours

$$\Gamma^\pm_a := \partial(\{\lambda \in \mathbb{C}^\pm : \operatorname{Re}(a\lambda^n) > 0\} \setminus \bigcup_{\substack{\sigma\in\mathbb{C};\\ \Delta(\sigma)=0}} D(\sigma, 2\epsilon)) \tag{3.4a}$$

$$\Gamma_a := \Gamma^+_a \cup \Gamma^-_a \tag{3.4b}$$

$$\Gamma^+_0 := \bigcup_{\substack{\sigma\in\operatorname{cl}\mathbb{C}^+;\\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \tag{3.4c}$$

$$\Gamma^-_0 := \bigcup_{\substack{\sigma\in\mathbb{C}^-;\\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \tag{3.4d}$$

$$\Gamma_0 := \Gamma^+_0 \cup \Gamma^-_0 \tag{3.4e}$$

$$\Gamma := \Gamma_0 \cup \Gamma_a. \tag{3.4f}$$

A sample contour is shown in Figure 3.

The Fokas transform pair is given by

$$F_\lambda : f(x) \mapsto F(\lambda) \quad F_\lambda(f) = \begin{cases} F^+_\lambda(f) & \text{if } \lambda \in \Gamma^+_0 \cup \Gamma^+_a, \\ F^-_\lambda(f) & \text{if } \lambda \in \Gamma^-_0 \cup \Gamma^-_a, \end{cases} \tag{3.5a}$$

$$f_x : F(\lambda) \mapsto f(x) \quad f_x(F) = \int_\Gamma e^{i\lambda x} F(\lambda)\, d\lambda,\ x \in [0,1], \tag{3.5b}$$

which allows computing the IBVP solution $q(x,t)$ in (1.7) by

$$\begin{aligned} q(x,t) &= f_x\left(e^{-a\lambda^n t} F_\lambda(f)\right) \\ &= \int_{\Gamma^+_0} e^{i\lambda x} e^{-a\lambda^n t} F^+_\lambda(f)\, d\lambda + \int_{\Gamma^+_a} e^{i\lambda x} e^{-a\lambda^n t} F^+_\lambda(f)\, d\lambda \\ &\quad + \int_{\Gamma^-_0} e^{i\lambda x} e^{-a\lambda^n t} F^-_\lambda(f)\, d\lambda + \int_{\Gamma^-_a} e^{i\lambda x} e^{-a\lambda^n t} F^-_\lambda(f)\, d\lambda. \end{aligned} \tag{3.6}$$

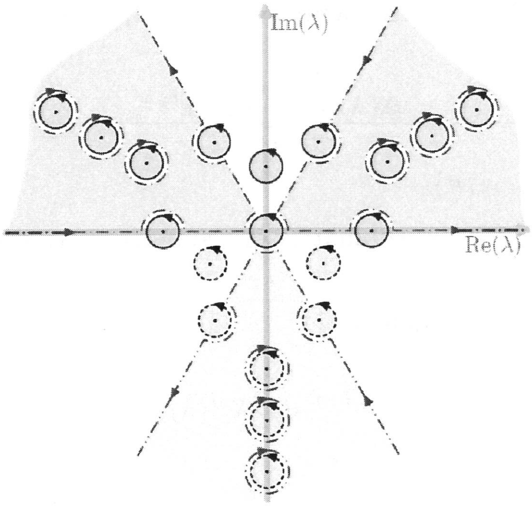

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Figure 3: Hypothetical Γ contours corresponding to the case $a = -i$, taken from [1]. The red dashed lines correspond to Γ_a^+, and the green dashed lines correspond to Γ_a^-. The blue circles correspond to Γ_0^+, and the black circles correspond to Γ_0^-. The arrows indicate the order of integration in equation (3.6).

3.2.1 Characterizing contours

All objects defined above except for the contour Γ, namely $W^+(\lambda)$, $W^-(\lambda)$, $W(\lambda)$, $\Delta(\lambda)$, X^{lj}, $F_\lambda^+(f)$, $F_\lambda^-(f)$, can be constructed directly from their explicit expressions. Thus, to construct the Fokas transform pair F_λ and f_x, we only need to find an explicit characterization of the contour Γ.

We note that by (3.4), Γ_a^+ and Γ_a^- are boundaries of the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ in the upper and lower half planes, respectively, deformed to avoid zeroes of $\Delta(\lambda)$. On the other hand, Γ_0^+ and Γ_0^- consist of circles of radius ϵ around zeroes of $\Delta(\lambda)$ in the closed upper half plane and the open lower half plane, respectively. Thus, to find Γ, we need to find the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ and the zeroes of $\Delta(\lambda)$.

Tracing contour sectors

We first find the region

$$\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}.$$

For $z \in \mathbb{C}$, define $\theta_z := \arg(z)$ and $r_z := |z|$. Let $\lambda \in \mathbb{C}$. Then

$$a\lambda^n = r_a e^{i\theta_a} \cdot r_\lambda^n e^{ni\theta_\lambda} = r_a r_\lambda^n e^{i(\theta_a + n\theta_\lambda)} = r_a r_\lambda^n (\cos(\theta_a + n\theta_\lambda) + i\sin(\theta_a + n\theta_\lambda)).$$

Thus,

$$\mathrm{Re}(a\lambda^n) = r_a r_\lambda^n \cos(\theta_a + n\theta_\lambda),$$

where

$$\mathrm{Re}(a\lambda^n) > 0 \iff \cos(\theta_a + n\theta_\lambda) > 0.$$

But

$$\cos(\theta_a + n\theta_\lambda) > 0 \iff \theta_a + n\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(2\pi k - \frac{\pi}{2}, 2\pi k + \frac{\pi}{2}\right),$$

and so

$$\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k - \frac{\pi}{2} - \theta_a}{n}, \frac{2\pi k + \frac{\pi}{2} - \theta_a}{n}\right).$$

Note that ~~by~~ the original infinite contour integrals must be understood as improper integrals which, whenever they exist, are equal to their principal values. Truncating within $D(0,d)$ and expecting convergence as $d \to \infty$ is therefore legitimate.

For example, when $a = -i$ and $n = 3$,

$$\theta_\lambda \in \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k - \frac{\pi}{2} - (-\frac{\pi}{2})}{3}, \frac{2\pi k + \frac{\pi}{2} - (-\frac{\pi}{2})}{3} \right) = \bigcup_{k\in\mathbb{Z}} \left(\frac{2\pi k}{3}, \frac{2\pi k + \pi}{3} \right).$$

Thus, in $[0, 2\pi)$,

$$\theta_\lambda = \arg(\lambda) \in \bigcup_{k\in\{0,1,2\}} \left(\frac{2\pi k}{3}, \frac{2\pi k + \pi}{3} \right) = \left(0, \frac{\pi}{3}\right) \cup \left(\frac{2\pi}{3}, \pi\right) \cup \left(\frac{4\pi}{3}, \frac{5\pi}{3}\right).$$

Figure 4 shows some simulations of the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$. Note that the region consists of individual segments, which we henceforth refer to as sectors.

Deforming contours

The boundaries of the sectors found above form the "backbones" of the contours Γ_a^+ and Γ_a^-. We proceed to turn these "backbones" into Γ_a^+, Γ_a^- by deforming them to avoid zeroes of $\Delta(\lambda)$.

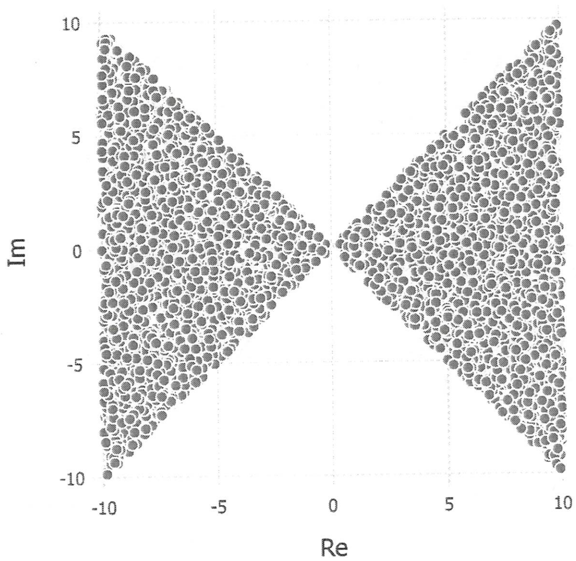
Before going into the technicalities of the contour deformation, we first draw attention to a modification of the mathematical construction of Γ in the actual implementation of the algorithm. In (3.4), Γ is defined on the entire complex plane; that is, we can have λ with arbitrarily large modulus. In the actual implementation, however, we choose a sufficiently large real number d to represent infinity in the algorithm's context. That is, we restrict the mathematical construction to the disk $D(0, d)$. As the choice of d potentially implies a tradeoff between computational cost and numerical accuracy, it should be chosen with regard to the error tolerance of the computational task at hand.

By the theory of exponential polynomials [9], $\Delta(\lambda)$ has infinitely many zeroes, yet any finite region contains only finitely many of these zeroes. Since we restrict the construction to the finite region $D(0, d)$, we would only be dealing with finitely many zeroes of $\Delta(\lambda)$. This is an important fact: One complication that arises in practice is that each circular contour around a zero of $\Delta(\lambda)$ not only cannot overlap with the circle around another zero but also cannot overlap with the boundary of any sector. That is, in Figure 3, the blue and black circles not only cannot overlap with each other, but they also cannot overlap with the red or green dashed lines if their centers lie exterior to the red or green sectors. This implies that the 5ϵ introduced in section 3.2 in fact needs to be the minimum of the infimum of the pairwise distances between distinct zeroes of $\Delta(\lambda)$ and the infimum of distances between each zero that is exterior to all sectors and the boundary of each sector. The theory of exponential polynomials [9] guarantees that the former infimum is positive, but there is no such guarantee for the latter infimum. However, precisely because we are working with a finite number of zeroes of $\Delta(\lambda)$ in $D(0, d)$, the latter infimum is positive, and so is ϵ.

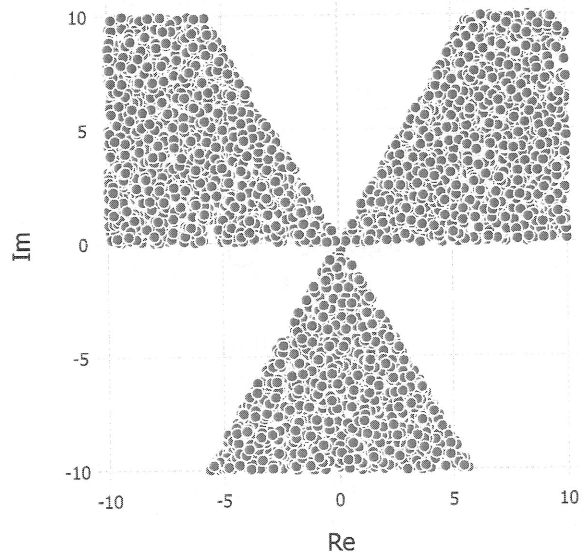
To see that our choice of ϵ is valid, suppose 5ϵ is the minimum of the two infim~~ums~~a described above. Then the circle of radius ϵ around a zero of $\Delta(\lambda)$ does not overlap with any sector boundary. Moreover, the contours around any two distinct zeroes of $\Delta(\lambda)$ do not overlap. Indeed: In Figure 5, suppose the radius of the blue circle around a zero of $\Delta(\lambda)$ is ϵ and the distance between the blue circle and the red dashed curve around it is again ϵ. Then since the distance between any two distinct zeroes of $\Delta(\lambda)$ is no less than 5ϵ, the blue circle together with the red dashed curve around it is still of distance $5\epsilon - 2\epsilon \cdot 2 = \epsilon$ from the red dashed curve and the blue circle surrounding the nearest zero of $\Delta(\lambda)$. Thus, our choice of ϵ ensures that no contour around a zero of $\Delta(\lambda)$ is "overwritten" by that around another.

Suppose for now that we have been given finitely many zeroes of $\Delta(\lambda)$ in $D(0, d)$ (we will show how to approximate these zeroes in the next section).

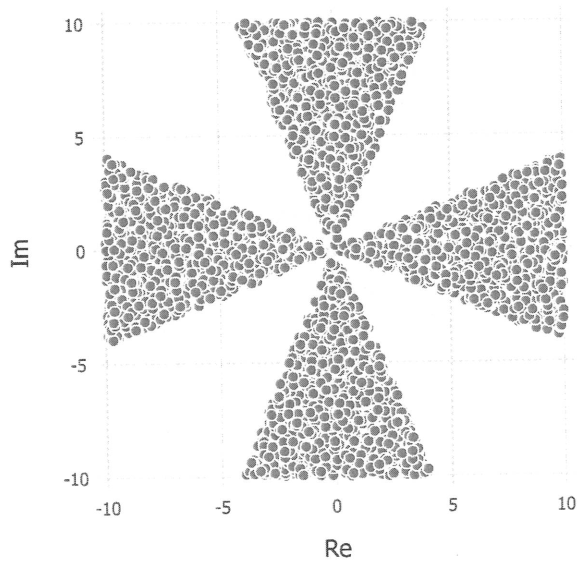
In the complex plane, ~~let~~ a ray (straight half-line) ~~going out~~ emanating from the origin ~~be~~ is characterized by the argument of any point on the ray. From Figure 4, we note that each sector in the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ is characterized by the arguments of the two rays that mark its



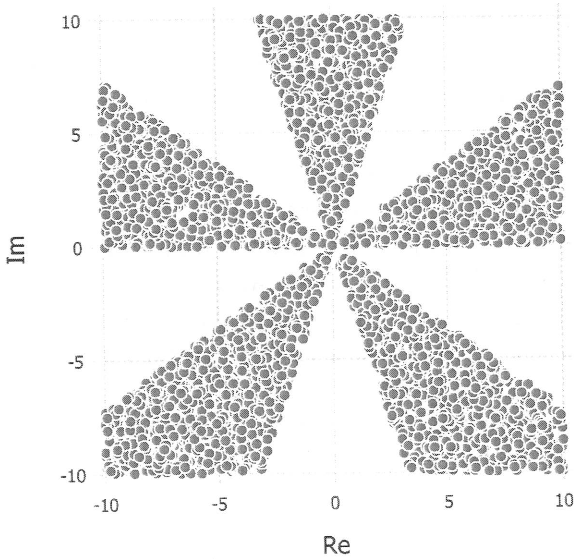
(a) $n = 2$, $a = 1$.



(b) $n = 3$, $a = -i$.



(c) $n = 4$, $a = 1$.



(d) $n = 5$, $a = -i$.

Figure 4: Simulation of the region $\{\lambda \in \mathbb{C} : \operatorname{Re}(a\lambda^n) > 0\}$ by randomly sampling 10^4 points λ and keeping those that satisfy $\operatorname{Re}(a\lambda^n) > 0$.

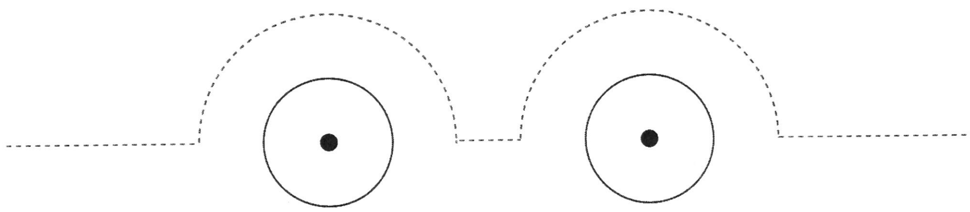


Figure 5: Two distinct zeroes of $\Delta(\lambda)$ that are 5ϵ apart. The blue circles and red dashed contours are as in Figure 3. The radius of the blue circles, the distance between each blue circle and the red dashed curve around it, and the distance between the two red dashed curves, are all ϵ.

boundaries, namely the starting ray and the ending ray, such that the if the sector is traversed counterclockwise from one end to the other, the starting ray will be traversed before the ending ray. For example, with $n = 3$ and $a = -i$, as shown in section 3.2.1, the region $\{\lambda \in \mathbb{C} : \mathrm{Re}(a\lambda^n) > 0\}$ is characterized by the rays with arguments $0, \frac{\pi}{3}, \frac{2}{3}\pi, \pi, \frac{4}{3}\pi, \frac{5}{3}\pi$, where $0, \frac{2}{3}\pi, \frac{4}{3}\pi$ are the angles of the starting rays, and $\frac{\pi}{3}, \pi, \frac{5}{3}\pi$ are the angles of the ending rays.

Note that each sector is assigned to Γ_a^+ or Γ_a^- depending on whether it belongs to the upper or the lower half plane. As shown in Figure 8, if a sector overlaps with the real line, we divide it into the upper and lower half planes, which can then be assigned to Γ_a^+ and Γ_a^-, respectively. In the implementation, this is done by modifying the starting and ending rays that characterize the sector so that it is split into two sub-sectors, one ending at the real line and the other starting at it.

The contours $\Gamma_a^\pm$ are built from these rays with possible deformations to avoid zeroes of $\Delta(\lambda)$. Here we make another modification of the mathematical construction in (3.4) to save computational cost. We note that the contours $\Gamma_a^\pm$ and $\Gamma_0^\pm$ defined in (3.4) lead to partial cancellation, and deformation is in fact only necessary if a zero lies on the boundary of some sector. Indeed: As illustrated in Figure 3, the red and blue dashed lines do not need to be deformed to avoid zeroes exterior to all sectors because they are already outside the sectors. Moreover, zeroes interior to any sector can be ignored, since integrating over the blue circle around the zero counterclockwise cancels with integrating over the interior red dashed circle around the zero clockwise. For a zero that lies on the boundary of the sector, half of the blue circle around it that is interior to the sector cancels out with the red dashed curve around it, but the other half that is exterior to the sector does not cancel with anything. In this case, we deform the ray on which the zero lies to include the half of the blue circle that does not cancel.

On a side note, the way we deform the contours described above implies that we can choose ϵ to be $\frac{1}{4}$ the minimum of the pairwise distances between distinct zeroes of $\Delta(\lambda)$ and the distances between any zero to any sector boundary, instead of $\frac{1}{5}$ as before. Indeed: Since we are merging the blue circle into the red dashed curve, the scenario in Figure 5 would not occur. Instead, the scenario that puts the most constraint on ϵ occurs when a zero is at the origin, and as shown in Figure 6, this scenario only requires that the two distinct zeroes are 4ϵ apart. Since zeroes of $\Delta(\lambda)$ are poles of F_λ^+, F_λ^- in (3.5a), the values of F_λ^+, F_λ^- may easily blow up near the zeroes, thereby creating numerical instability. Thus, we use the new choice of ϵ in the actual implementation to make the contours stay further away from the zeroes. Figure 7 shows the contour Γ for some examples, and Figure 8 shows each component of Γ of Figure 7(a) separately.

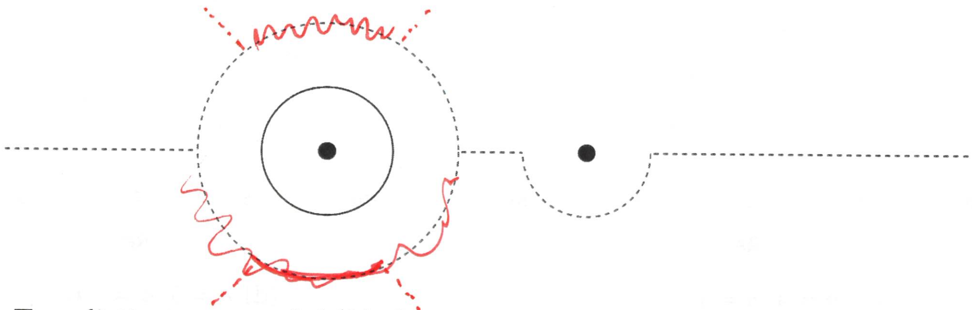
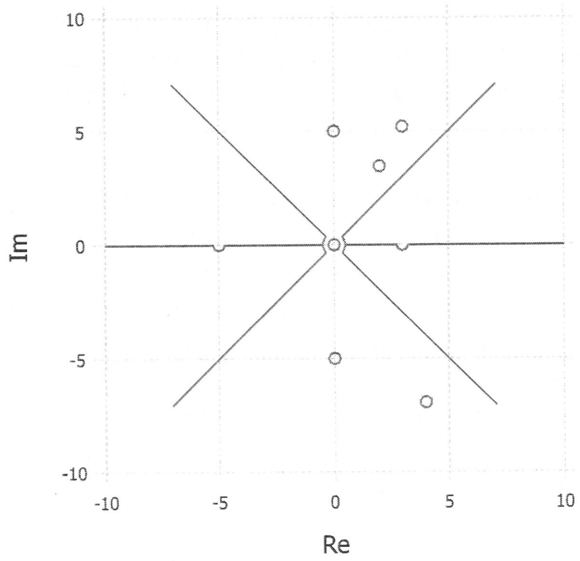
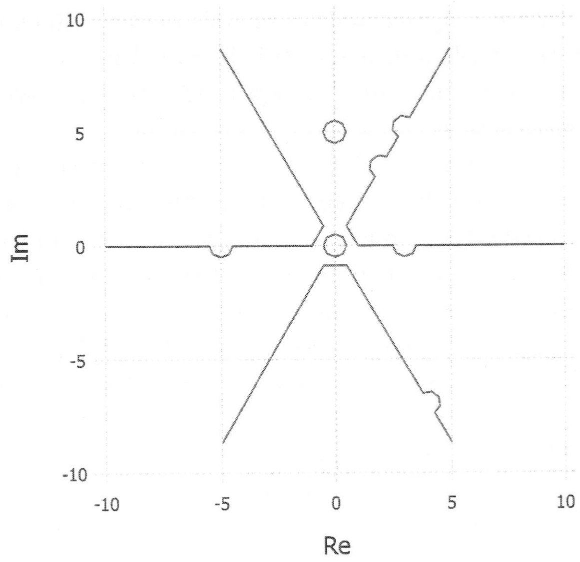


Figure 6: Two distinct zeroes of $\Delta(\lambda)$ that are 4ϵ apart. The zero on the left is at the origin. The blue circles and red dashed contours are as in Figure 3. The radius of the blue circles, the distance between the blue circle and the red dashed curve around it, and the distance between the two red dashed curves, are all ϵ.

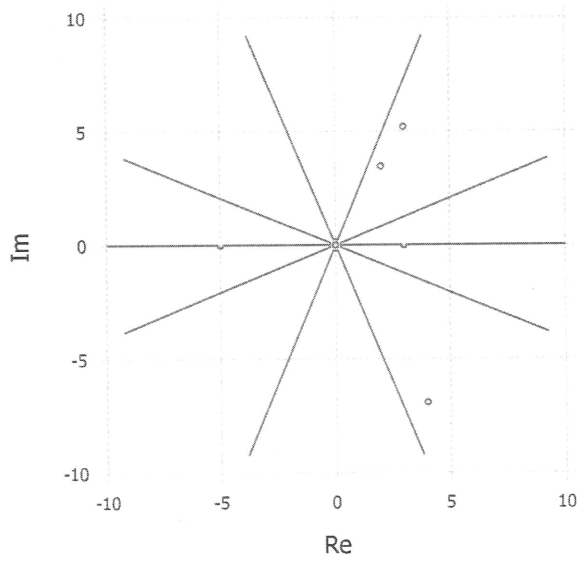
The construction of Γ_a^+, Γ_a^-, Γ_0^+, and Γ_0^- is described as follows. In the implementation, each contour in Γ is encoded by an array of points listed in the order of integration. By Figure 3, we integrate over each contour in $\Gamma_a^\pm$ from the ending ray to the starting ray, and each contour in $\Gamma_0^\pm$ counterclockwise. Thus, in constructing the contours, for each sector, we initialize its boundary contour by an array of three points, namely the point on the ending ray with distance



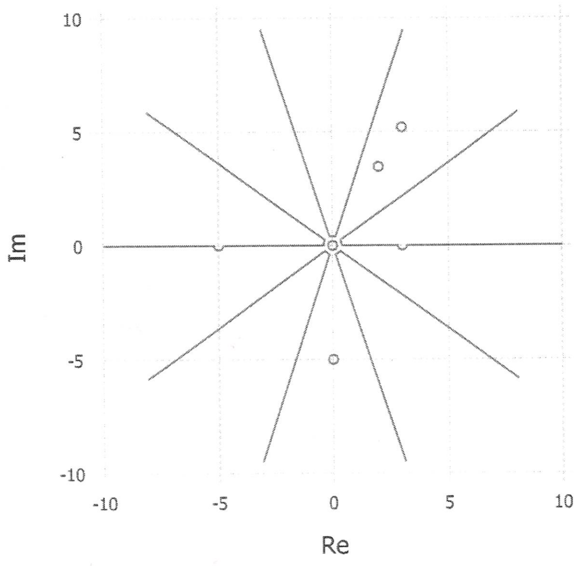
(a) $n=2$, $a=1$.



(b) $n=3$, $a=-i$.

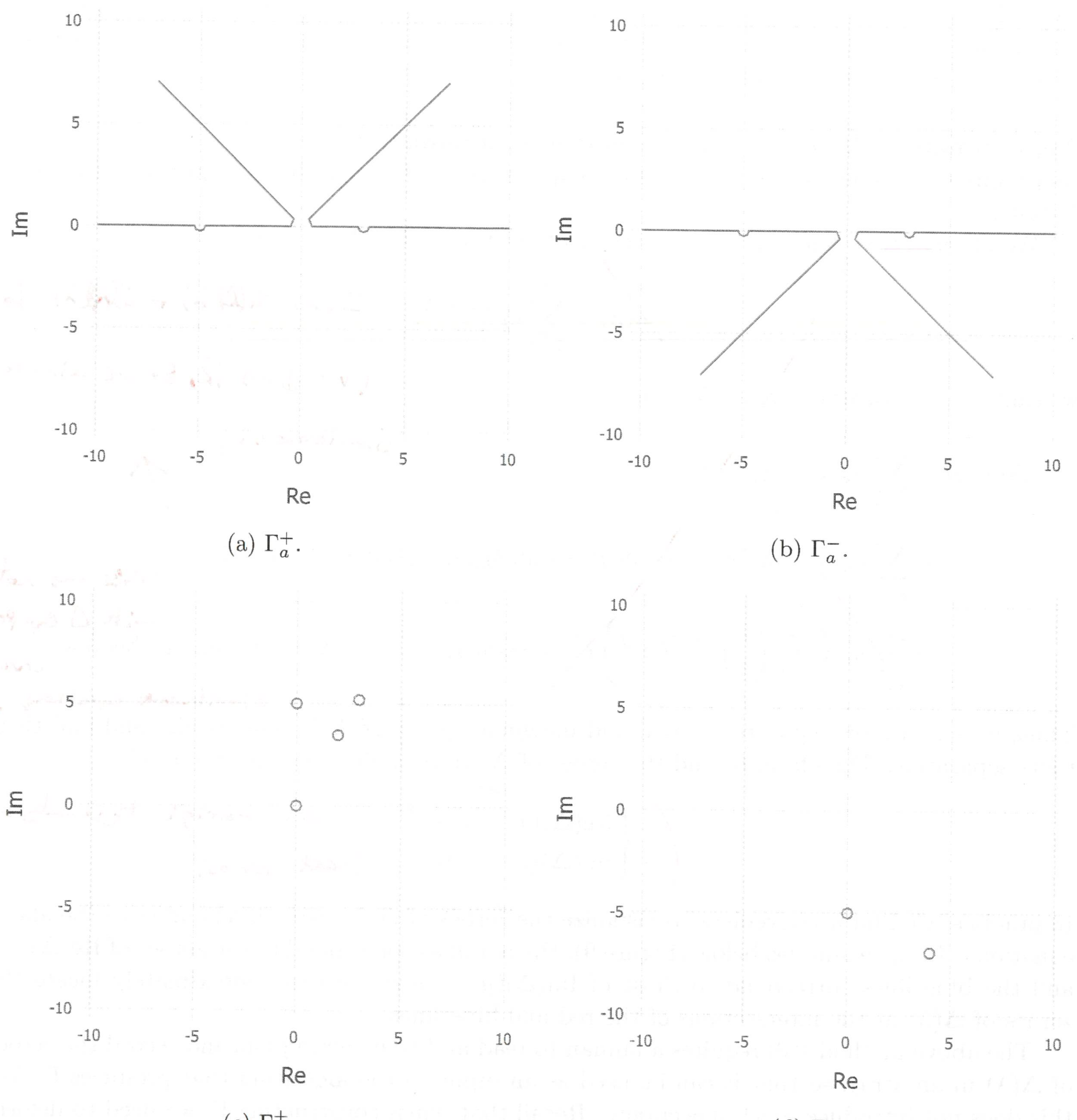


(c) $n=4$, $a=1$.



(d) $n=5$, $a=-i$.

Figure 7: Γ with with zeroes of $\Delta(\lambda)$ at $3+3\sqrt{3}i$, $2+2\sqrt{3}i$, $0+0i$, $0+5i$, $0-5i$, 3, -5, and $4-4\sqrt{3}i$. Note that Γ_a^+ are deformed to avoid zeroes on the sectors' boundaries.



(a) Γ_a^+.

(b) Γ_a^-.

(c) Γ_0^+.

(d) Γ_0^-.

Figure 8: Components of Γ with $n = 2$, $a = 1$, and the same zeroes of $\Delta(\lambda)$ as in Figure 7. Note that the sectors are split at the real line into the upper and lower half planes.

itself

d from the origin, the origin, and the point on the starting ray with modulus d. We add these initial sector boundary contours to $\Gamma_a^{\pm}$ depending on whether the sectors are in the upper or lower half planes. Then, for each zero of $\Delta(\lambda)$ that is not at the origin, if it is on the boundary of some sector, we deform the boundary contour of that sector to include a "bulge" that is the exterior half of an N-gon of radius ϵ around the zero, with the vertices listed counterclockwise. If the zero is exterior to all sectors, we add an N-gon contour around it to $\Gamma_0^{\pm}$, depending on whether the zero is in the upper or lower half plane. If the zero is interior to any sector, we ignore it, since its contribution to the contour integral will be cancelled out, as explained before. Finally, if there is a zero at the origin, we draw an N-gon around it and deform the boundary contours of all sectors to avoid the N-gon.

Approximating the roots of an exponential polynomial

As promised, we now describe a method to approximate the roots of $\Delta(\lambda)$ in the finite region $D(0, d)$.

We observe that since $\Delta(\lambda)$ is an exponential polynomial of the form

$$\Delta(\lambda) = \sum_{k=1}^{n} a_k \lambda^k e^{b_k \lambda},$$

$\Delta(\lambda) = \mathrm{Re}(\Delta)(\lambda) + i\,\mathrm{Im}(\Delta)(\lambda)$ for $u, v : \mathbb{C} \to \mathbb{R}$. So we aim to solve simultaneously

writing $\lambda = x + iy$ where $x, y \in \mathbb{R}$ gives

$$\begin{aligned}
\Delta(x,y) &= \sum_{k=1}^{n} a_k (x+iy)^k e^{b_k(x+iy)} \\
&= \sum_{k=1}^{n} a_k (x+iy)^k e^{b_k x}(\cos(b_k y) + i\sin(b_k y)) \quad \text{(Euler's formula)} \\
&= \sum_{k=1}^{n} a_k \left(\sum_{l=0}^{k} \binom{k}{l} x^{k-l} (iy)^l \right) e^{b_k x}(\cos(b_k y) + i\sin(b_k y)) \quad \text{(Binomial theorem).}
\end{aligned}$$

This has nothing to do with Δ exp poly, and, crucially, in the simultaneous equations, $x, y \in \mathbb{C}$ not $x, y \in \mathbb{R}$.

Thus, we can always separate the real and imaginary parts of $\Delta(\lambda)$ analytically and find their roots separately. Therefore, to find the zeroes of $\Delta(\lambda)$, it suffices to solve for x, y in

$$\begin{cases} \mathrm{Re}(\Delta)(x) &= 0, \\ \mathrm{Im}(\Delta)(y) &= 0. \end{cases}$$

I am worried this only finds real zeros.

In practice, we find it convenient to visualize the zeroes of $\Delta(\lambda)$ using level curves of the above equations. In the examples below (Figure 9), the red lines correspond to the zeroes of $\mathrm{Re}(\Delta)(x)$, and the blue lines correspond to those of $\mathrm{Im}(\Delta)(y)$. Thus, we can approximately locate the zeroes of $\Delta(\lambda)$ at the intersections of the red and blue lines.

The above method still requires a human to read and level curve plots and record the zeroes of $\Delta(\lambda)$ in an array, so that it can be used as an input to the algorithm that produces Γ. Yet this does not introduce much inaccuracy: Recall that when constructing Γ, we need to deform the contours to avoid zeroes of $\Delta(\lambda)$ with N-gons of radius ϵ. Thus, there is relatively high tolerance for our approximation of the locations of the zeroes.

3.2.2 Approximating Integral Using Chebyshev Polynomials

With the above contour construction, theoretically, we can already compute the Fokas transform pair F_λ and f_x and solve for $q(x,t)$. Yet there is one more complication in practice. As shown in equation (3.6), the definition of the solution $q(x,t)$ involves integration of F_λ^+, F_λ^- over the Γ contours, but as shown in (3.3a) – (3.3b), F_λ^+ and F_λ^- themselves involve an integral of the initial data $f(x)$. Double integrals are computationally expensive, and so to improve algorithm