Fast expansion on the real line

Helge Dietert[*] Arieh Iserles[†]

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Abstract

Fast approximation of functions on the real line is a key to a long list of applications, not least to the use of spectral methods for PDEs with Cauchy boundary conditions: our particular interest is in equations of quantum mechanics, when the solution behaves like a linear combination of wave packets. A longstanding goal is to approximate such functions with either Hermite polynomials or Hermite functions. In this paper we present such an algorithm, yet claim that Hermite expansions are unsuitable in the case of wave packets. Instead we recommend stretched Fourier expansions, an intermediate stage in our Hermite expansion algorithm. Although functions under consideration are not periodic, we prove that stretched Fourier expansions converge at a spectral speed once the 'window' of approximation is suitably chosen.

1 Motivation

Spectral methods are an extraordinarily effective tool in the computation of partial differential equations (PDEs) and the reason is twofold. Firstly, orthogonal expansions of sufficiently smooth functions converge very rapidly. Given for the sake of simplicity a linear PDE $\mathcal{L}u = f$ (where $\mathcal{L}$ contains space, and perhaps also time, derivatives) we approximate $u \approx \sum_{m=0}^{n-1} a_m \varphi_m$, where $\Phi = \{\varphi_m\}_{m\geq 0}$ is a dense orthogonal system in the underlying Hilbert space $\mathcal{H}$. The unknowns are $a_0, \ldots, a_{n-1}$ and they can be expressed as a solution of an $n \times n$ linear algebraic system. Because of rapid convergence, we can choose relatively modest value of n, rendering the solution fairly affordable.

Secondly, for several important orthogonal systems Φ and an arbitrary $h \in \mathcal{H}$, we can compute the first n coefficients $\hat{h}_m$, such that $h = \sum_{m=0}^{\infty} \hat{h}_m \varphi_m$, in $\mathcal{O}(n \log_2 n)$ operations.

The most important example is $\mathcal{H} = \mathrm{L}^2_{\mathrm{per}}[-\pi, \pi]$, the set of square-integrable functions in $[-\pi, \pi]$ with periodic boundary conditions. In that case, setting $\varphi_{2m}(x) = \mathrm{e}^{\mathrm{i}mx}$ and $\varphi_{2m+1}(x) = \mathrm{e}^{-\mathrm{i}mx}$, $m \geq 0$ (in other words, a Fourier expansion) we can compute the first n coefficients with Fast Fourier Transform (FFT) in $\mathcal{O}(n \log_2 n)$

[*]Institut de Mathématiques de Jussieu – Paris Rive Gauche (IMJ-PRG), Université Paris 7 Denis Diderot – Sorbonne Paris Cité, 75205 Paris CEDEX 13, France.

[†]Department of Applied Mathematics and Theoretical Physics (DAMTP), University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, UK.

operations. This can be easily extended to expansions in Chebyshev polynomials T_m, $m \geq 0$, whose closure is $\mathrm{L}^2[-1,1]$, thereby allowing for Dirichlet boundary conditions. Other polynomial expansions are based in the main on first expanding in Chebyshev polynomials, subsequently converting to another polynomial orthogonal basis: in order of increased generality Legendre polynomials (Hale & Townsend 2016, Iserles 2011, Potts, Steidl & Tasche 1998), ultraspherical polynomials (Cantero & Iserles 2012) and Jacobi polynomials (Wang & Huybrechs 2014). (One should also mention an alternative means of computing a Legendre expansion in $\mathcal{O}\big(n(\log_2 n)^2\big)$ operations using the fast multipole method (Alpert & Rokhlin 1991).)

The main purpose of this paper is to extend the realm of orthogonal systems whose first n coefficients can be computed rapidly to the real line. Many PDEs are originally stated in $\mathbb{R}^d$ with Cauchy boundary conditions. Yet, for the purpose of numerical solution they are often restricted to a compact domain $\Omega \subset \mathbb{R}^d$, a procedure that requires a great deal of ingenuity: Dirichlet-to-Neumann maps, absorbing or reflecting boundary conditions etc. In particular, we are motivated by equations of quantum mechanics in the semiclassical regime. A typical example (and the primary motivation for this work) is the time-dependent linear Schrödinger equation

$$\frac{\partial u}{\partial t} = \mathrm{i}\epsilon\Delta u - \mathrm{i}\epsilon^{-1}V(\boldsymbol{x},t)u, \tag{1.1}$$

where $u = u(\boldsymbol{x},t)$ with $\boldsymbol{x} \in \mathbb{R}^d$, $t \geq 0$ and $\epsilon > 0$ is a small parameter. The equation (1.1) describes the motion of a particle in an electric field governed by the potential V. Solving (1.1), the domain is usually restricted to $[-a,a]^d$, accompanied by periodic boundary conditions, and the standard justification rests upon three assumptions. Firstly, quantum systems typically persist in a semiclassical regime only for limited time; secondly, practical methods can be employed only for short time; and, thirdly, typical solution is a linear combination of *Hagedorn wave packets*

$$\exp\left(\frac{\mathrm{i}}{2\epsilon}(\boldsymbol{x}-\boldsymbol{x}_0)^\top PQ^{-1}(\boldsymbol{x}-\boldsymbol{x}_0) + \frac{\mathrm{i}}{\epsilon}\boldsymbol{p}^\top(\boldsymbol{x}-\boldsymbol{x}_0)\right), \tag{1.2}$$

where P and Q are $d \times d$ complex nonsingular matrices such that $Q^\top P = P^\top Q$ and $Q^*P - P^*Q = 2\mathrm{i}I$: hence PQ^{-1} is complex symmetric and $\operatorname{Im} PQ^{-1} = (QQ^*)^{-1}$ Hermitian and positive definite (Faou, Gradinaru & Lubich 2009, Jin, Markowich & Sparber 2011, Lasser & Troppmann 2014). Moreover, the initial condition is a linear combination of a small number of wave packets. Therefore, the solution is highly localised and remains so for some time. Provided that $a > 0$ is large enough, it matters little what are the boundary conditions at $\pm a$ and the most convenient course of action is to impose periodicity.

The first two assumptions are challenged by recent developments in quantum control and in numerical analysis. Firstly, it is possible to manipulate and control particles by a judicious use of short-burst laser pulses (Kosloff, Rice, Gaspard, Tersigni & Tannor 1998, Shapiro & Brumer 2003) and, secondly, a new breed of numerical methods allows for effective computation of (1.1) for very long time intervals (Bader, Iserles, Kropielnicka & Singh 2014, Bader, Iserles, Kropielnicka & Singh 2016). The practical consequence is that, unless $a > 0$ is very large (thereby increasing the cost), sooner or later the solution is likely to break down due to boundary effects. The standard remedy, replacing a Fourier by a Chebyshev basis, is not open to us because an essential structural feature of (1.1), which must be preserved under discretisation, is the conservation of L^2 norm, and this cannot be done with any polynomial basis.[1] A far better course of action is to abandon altogether the restriction to $[-a,a]^d$ and solve (1.1) in $\mathbb{R}^d$. This was the original motivation for this paper but we mention in passing that many other PDEs, not just in quantum mechanics, are ideally solved in $\mathbb{R}^d$.

The most obvious basis in $\mathbb{R}$ (which can be extended to $\mathbb{R}^d$ by tensor products) consists of *Hermite polynomials* H_m: each H_m is a polynomial of degree m,

$$\langle \mathrm{H}_m, \mathrm{H}_n \rangle_{\mathsf{P}} = 0, \quad m \neq n, \qquad \text{where} \qquad \langle f, g \rangle_{\mathsf{P}} = \int_{-\infty}^{\infty} f(x)\bar{g}(x)\mathrm{e}^{-x^2}\,\mathrm{d}x \tag{1.3}$$

and $\langle \mathrm{H}_m, \mathrm{H}_m \rangle_{\mathsf{P}} = \pi^{1/2}2^m m!$ (DLMF 2016, 18.3). Alternatively, we might contemplate *Hermite functions*

$$\psi_m(x) = \frac{(-1)^m}{(\pi^{1/2}2^m m!)^{1/2}}\mathrm{e}^{-x^2/2}\mathrm{H}_m(x), \qquad m \geq 0 \tag{1.4}$$

(Fedoryuk 2001). It follows at once from (1.3) that

$$\langle \psi_m, \psi_n \rangle_{\mathsf{F}} = \begin{cases} 1, & m = n, \\ 0, & m \neq n, \end{cases} \qquad \text{where} \qquad \langle f, g \rangle_{\mathsf{F}} = \int_{-\infty}^{\infty} f(x)\bar{g}(x)\,\mathrm{d}x$$

is the standard inner product on $\mathrm{L}^2(\mathbb{R})$. The choice of Hermite functions is natural in the context of quantum mechanics because $\psi_n'' + (2m+1-x^2)\psi_m = 0$, therefore they are eigenfunctions of the Schrödinger operator with harmonic potential. Even more importantly in our context, since (letting $\psi_{-1} \equiv 0$)

$$\psi_m' = \left(\frac{m}{2}\right)^{1/2}\psi_{m-1} - \left(\frac{m+1}{2}\right)^{1/2}\psi_{m+1}, \qquad m \geq 0,$$

their differentiation matrix is skew symmetric and tridiagonal. (Clearly, the differentiation matrix of Hermite – or any other – polynomials cannot be skew symmetric.) Skew symmetry of a differentiation matrix confers important advantages for numerical stability and conservation of energy (Hairer & Iserles 2016). Another welcome feature of Hermite functions is that they are uniformly bounded: according to the *Cramér inequality* $|\psi_m(x)| \leq K\pi^{-1/4}$, where $K \approx 1.0864$, for all $m \geq 0$ and $x \in \mathbb{R}$ (Szegő 1955). Finally, Hermite function expansions converge for a large set of functions of interest (Boyd 1980).

Unfortunately, both Hermite polynomials and Hermite functions have major drawbacks. Hermite polynomials become rapidly large for large m or $|x|$:

$$\mathrm{H}_{2m}(0) = (-1)^m\frac{(2m)!}{m!}, \qquad \mathrm{H}_m(x) \sim (2x)^m, \quad |x| \gg 1$$

[1] It is possible to use ultraspherical polynomials while conserving energy (Townsend & Olver 2015), but this does not coexist with other crucial features of the methods from (Bader et al. 2014, Bader et al. 2016).

(DLMF 2016, 18.5.13). Therefore, even once expansion coefficients decay very rapidly, the expansion itself, being a sum of products of very small and very large numbers, is numerically unstable. Hermite functions are stable, since the ψ_ms are uniformly bounded, yet both expansions have another downside insofar as wave packets are concerned. To get a general impression what we can expect from Hermite expansions of wave packets, we have considered a function

$$f(x) = \mathrm{e}^{-x^2}\cos(20x)$$

– it oscillates within the envelope yet this oscillation is relatively mild insofar as (1.2) is concerned. The function is displayed in Fig. 1.1 in the interval $[-10, 10]$.

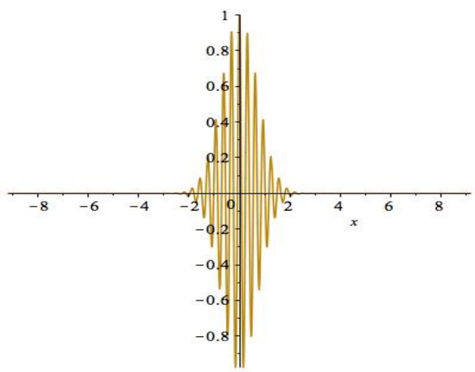

Figure 1.1: The wave packet $f(x) = \mathrm{e}^{-x^2}\cos(20x)$.

We have expanded f in *normalised Hermite polynomials*

$$\check{\mathrm{H}}_m(x) = \frac{\mathrm{H}_m(x)}{(\pi^{1/2}2^m m!)^{1/2}}, \qquad m \geq 0,$$

(hence $\langle \check{\mathrm{H}}_m, \check{\mathrm{H}}_m \rangle_{\mathsf{P}} \equiv 1$ and the system is orthonormal – compare with (1.4)) and in Hermite functions. The even coefficients, $\hat{f}_m^{\mathsf{P}}$ and $\hat{f}_m^{\mathsf{F}}$, respectively, are displayed in logarithmic scale in Fig. 1.2. (The odd coefficients are nil, since f is an even function.) It is clear that the coefficients range across many orders of magnitude and it is equally clear that we require quite a large number of coefficients for convergence. We reiterate that this f is just a toy example: in reality oscillation is likely to be significantly more rapid, with obvious implication on the rate of convergence.

Instead of either Hermite polynomials or functions, we advocate in this paper an alternative approach, that of *stretched Fourier expansions.* Before we explain this (fairly simple) idea, in Fig. 1.3 we display (in a similar manner to Fig. 1.2) stretched Fourier expansion coefficients greater than 10^{-20}: it is clear that there are *far* fewer of them and that the convergence occurs at spectral speed! This advantage grows rapidly with more rapid oscillation.

A stretched Fourier expansion is a standard Fourier expansion scaled to an interval

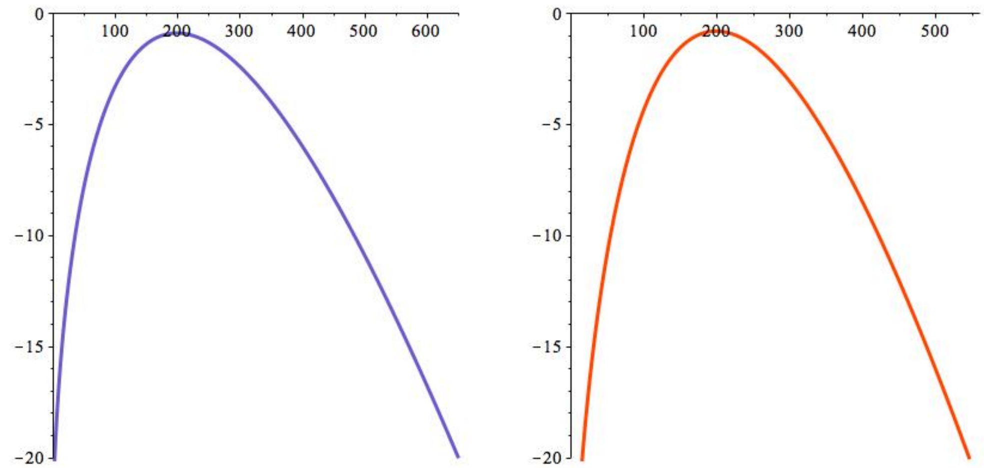

Figure 1.2: $\log_{10}|\hat{f}^{\mathsf{P}}_m|$ (on the left) and $\log_{10}|\hat{f}^{\mathsf{F}}_m|$ for even m and coefficients greater than 10^{-20} in magnitude.

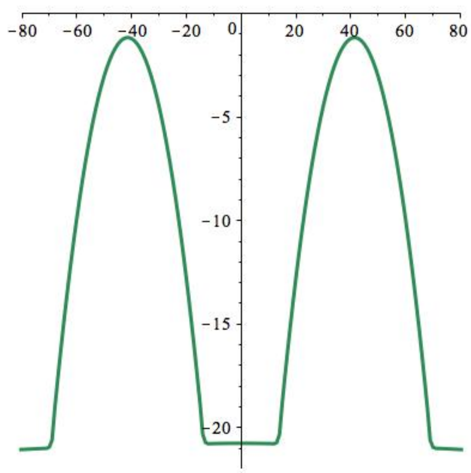

Figure 1.3: $\log_{10}|\hat{f}^{\lambda}_m|$ for stretched Fourier expansion with $\lambda \approx 6.5044$ and coefficients greater than 10^{-20} in magnitude.

$[-\lambda, \lambda]$, with a carefully chosen $\lambda > 1$, in other words

$$f(x) = \sum_{m=-\infty}^{\infty} \hat{f}^{\lambda}_m \mathrm{e}^{\mathrm{i}\pi m x/\lambda}, \qquad \text{where} \qquad \hat{f}^{\lambda}_m = \frac{1}{2\lambda}\int_{-\lambda}^{\lambda} f(x)\mathrm{e}^{-\mathrm{i}\pi m x/\lambda}\,\mathrm{d}x, \quad m \in \mathbb{Z}.$$

Needless to say, the truncated expansion can be computed fast with FFT.

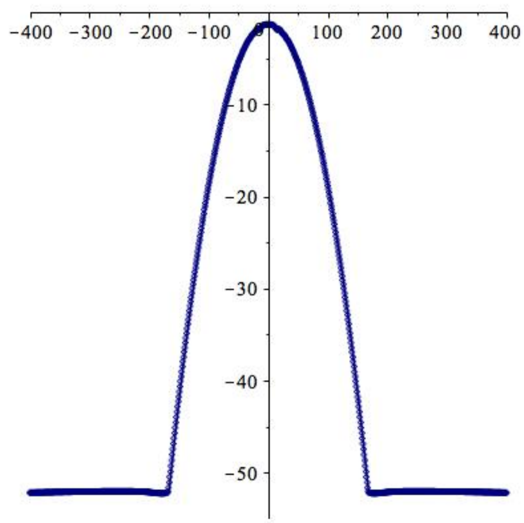

Figure 1.4: $\log_{10}|\hat{f}_n^\lambda|$ for $f(x) = \mathrm{e}^{-x^2/2}\cos(x^2 - x)$ with $\lambda = 15$.

The obvious objection to this procedure is that f is in general not periodic. Thus, even if $f \in \mathrm{C}^\infty(\mathbb{R})$, all we can hope for is linear decay of the coefficients, i.e. $|\hat{f}_m^\lambda| \approx c/|m|$ for $|m| \gg 1$ and some $c > 0$. Like many statements in mathematics, this is entirely true but, in the current context, totally misleading...

Examine again Fig. 1.3: the coefficients decay at spectral speed, essentially $|\hat{f}_m^\lambda| \approx c\,\mathrm{e}^{-\beta|m|^2}$ for sufficiently large $|m|$ and $c, \beta > 0$. This is not a paradox! Spectral decay does not persist for ever but, once it stops, the coefficients are negligibly small and can be disregarded. The secret lies in f decaying rapidly (as, for example, wave packets do!) for $|x| \gg 1$. To illustrate this point, we consider in Fig. 1.4 the function $\mathrm{e}^{-x^2/2}\cos(x^2 - x)$ in the 'window' $[-\lambda, \lambda]$, where $\lambda = 15$. The coefficients commence by decaying *at a spectral speed,* and they do so until they are $\approx 10^{-53}$ in magnitude: only then they behave 'according to the theory'. Given that 10^{-53} is well beyond the accuracy required in real-life numerical computation, to all practical intents and purposes the coefficients decay at a spectral speed!

In Section 2 we analyse this 'sombrero effect', a name originating in the shape of the curve in Fig. 1.4, for different types of functions that exhibit rapid decay for $|x| \gg 1$ and discuss how to choose λ adroitly, to ensure that we approximate spectrally fast within a relevant range. A subtle side issue is the effect on the Discrete Fourier Transform (DFT) calculation of Fourier coefficients of trading off periodicity for rapid decay. In Appendix A we demonstrate that within the spectral decay regime the DFT error is also exponentially small.

Section 3 shows how to 'lift' a stretched Fourier expansion to an expansion in either Hermite polynomials or Hermite functions. Although we have argued that such expansions are probably unsuitable for calculations of wave packets and quantum phenomena, this does not mean that they have no place in numerical analysis. For example, expansion in Hermite polynomials is critical in computations involving fast Gauss transform (Greengard & Strain 1991). We are not aware of any reasonable numerical algorithm for the computation of general Hermite expansions except for a laborious (and very expensive) use of Hermite integration with suitably large number of points, hence the work of Section 3 might be of an interest. Finally, in Section 4 we revisit the results of this paper and sketch challenges for future work.

2 Fourier expansion of stretched functions

2.1 The sombrero lemmas

Given $f \in \mathbb{C}^\infty(\mathbb{R})$ and $\lambda > 1$, we Fourier expand f in the interval $[-\lambda, \lambda]$. In other words, the Fourier coefficients are

$$\hat{f}_m^\lambda = \frac{1}{2\lambda} \int_{-\lambda}^{\lambda} f(x) \mathrm{e}^{-\mathrm{i}m\pi x/\lambda} \, \mathrm{d}x = \frac{1}{2} \int_{-1}^{1} f(\lambda x) \mathrm{e}^{-\mathrm{i}m\pi x} \, \mathrm{d}x, \qquad m \in \mathbb{Z}. \tag{2.1}$$

This is the moment to remind the reader that Fourier expansions are a very powerful and popular tool in scientific computing because a Fourier integral, under fairly generous conditions, can be computed to exponential accuracy by a Discrete Fourier Transform: using the Fast Fourier Transform (FFT), this 'costs' just $\mathcal{O}(N \log_2 N)$ operations for computation of $\hat{f}_m^\lambda$, $-N+1 \le m \le N$ (Henrici 1979).

Making no assumptions whatsoever on periodicity, all we can say by this stage about the asymptotic behaviour of the sequence $\{\hat{f}_m^\lambda\}_{m=-\infty}^{\infty}$ is that there exists $c_\lambda > 0$, which depends on f, such that

$$|\hat{f}_m^\lambda| \sim \frac{c_\lambda}{|m|}, \qquad |m| \gg 1. \tag{2.2}$$

While formally true, this is misleading, provided that f decays sufficiently rapidly for large $|x|$. To make our case we call in evidence Figs 1.4 and 2.1. Thus, Fig. 2.1 reports the size of Fourier coefficients for three functions: the first is entire, the second is analytic with poles at $\pm\mathrm{i}$ and the third analytic with a single pole at $+\mathrm{i}$. The first plot is similar to Fig. 1.4: the coefficients decay at higher-than-exponential speed until they hit a 'floor', along which the decay is consistent with (2.2) with $c_{15} \approx 1.71 \times 10^{-49}$. In the middle figure f is meromorphic and the decay of the $|f_m^\lambda|$s is exponentially fast until it hits the 'floor': this time $c_{15} \approx 1.99 \times 10^{-53}$. Finally, the function on the right has a singularity at the upper half plane only. Now the decay is exponential for $m \ll -1$ and super-exponential for $m \gg 1$ – until again we hit the 'floor', this time at $c_{15} \approx 2.92 \times 10^{-51}$. Note that the different values of c_{15} are in the same ballpark, indicating that the dependence of c_λ is mainly on the size of λ, rather than on a specific function f.

Our observations are presented in four lemmas, in an increasing extent of smoothness of the function f.

Lemma 1 *Let $\lambda > 1$ and $f \in \mathrm{C}^N[-\lambda, \lambda]$ be given, where $N \ge 1$. Then*

$$|\hat{f}_m^\lambda| \le \frac{1}{2\pi m} \sum_{\ell=0}^{N-1} \left(\frac{\lambda}{\pi m}\right)^\ell \delta + \left(\frac{\lambda}{\pi m}\right)^N \kappa, \qquad m \neq 0, \tag{2.3}$$

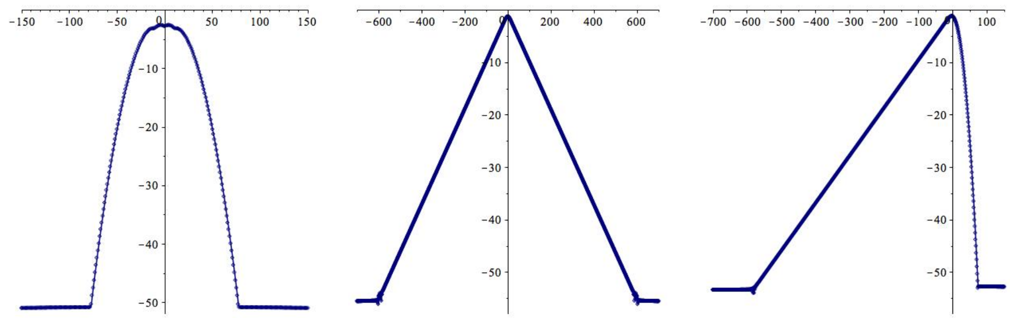

Figure 2.1: $\log_{10}|\hat{f}_m^\lambda|$ for (from the left) $f(x) = \mathrm{e}^{-x^2/2}(\cos x + x^2 \sin x)$, $f(x) = \mathrm{e}^{-x^2/2}/(1+x^2)$ and $f(x) = \mathrm{e}^{-x^2/2}/(1+\mathrm{i}x)$, all with $\lambda = 15$.

where $\kappa = \|f^{(N)}\|_\infty = \max_{x\in[-\lambda,\lambda]} |f^{(N)}(x)|$ *and*

$$\delta = \max_{j=0,\ldots,N-1} \max\{|f^{(j)}(-\lambda)|, |f^{(j)}(\lambda)|\}.$$

Proof Trivial. By repeated integration by parts we have

$$\hat{f}_m^\lambda = -\frac{(-1)^m}{2\lambda}\sum_{\ell=0}^{N-1}\left(\frac{\lambda}{\mathrm{i}\pi m}\right)^{\ell+1}[f^{(\ell)}(\lambda) - f^{(\ell)}(-\lambda)]$$
$$+\frac{1}{2\lambda}\left(\frac{\lambda}{\mathrm{i}\pi m}\right)^N \int_{-\lambda}^{\lambda} f^{(N)}(x)\mathrm{e}^{-\mathrm{i}\pi m x/\lambda}\,\mathrm{d}x$$

and the lemma follows by easy majorization. □

The importance of (2.3) is that the upper bound is composed of two terms: for $|m| > \lambda/\pi$ they are

$$\frac{1-\left(\frac{\lambda}{\pi m}\right)^N}{2(\pi m - \lambda)}\delta \qquad \text{and} \qquad \left(\frac{\lambda}{\pi m}\right)^N \kappa.$$

The second term decays rapidly, like $\mathcal{O}(m^{-N})$, while the first term is small once f and its derivatives are small at $\pm\lambda$.

We can formulate a sharper result for an analytic f.

Lemma 2 *Given* $r > 0$*, suppose that an analytic function* $f : [-\lambda, \lambda] \to \mathbb{C}$ *can be continued analytically to the closed rectangle*

$$\mathcal{S}_r = \{z \in \mathbb{C} : \mathrm{Re}\, z \in [-\lambda, \lambda],\ \mathrm{Im}\, z \in [-r, r]\}.$$

Define

$$\sigma = \max_{x\in[-\lambda,\lambda]} \max\{|f(x-\mathrm{i}r)|, |f(x+\mathrm{i}r)|\} \ \textit{and}\ \rho = \max_{y\in[-r,r]} \max\{|f(-\lambda+\mathrm{i}y)|, |f(\lambda+\mathrm{i}y)|\}.$$

Then

$$|\hat{f}_m^\lambda| \le \sigma \mathrm{e}^{-(\pi r/\lambda)|m|} + \frac{\rho}{\pi|m|}, \qquad m \neq 0. \tag{2.4}$$

Proof The boundary of $\mathcal{S}_r$ is a union of six contours,

$$\Gamma_1^{\pm} = \{-\lambda \pm \mathrm{i}y \,:\, 0 \le y \le r\}, \qquad \Gamma_2^{\pm} = \{x \pm \mathrm{i}r \,:\, -\lambda \le x \le \lambda\}$$

and

$$\Gamma_3^{\pm} = \{\lambda \pm \mathrm{i}y \,:\, 0 \le y \le r\}.$$

Let $m \ge 1$. By the Cauchy integral theorem,

$$\hat{f}_m = I_1 + I_2 + I_3, \quad \text{where} \quad I_j = \frac{1}{2\lambda}\int_{\Gamma_j^-} f(z)\mathrm{e}^{-\mathrm{i}\pi m z/\lambda}\,\mathrm{d}z, \quad j = 1,2,3.$$

(We need to endow the Γ_j^-s with orientation, but this makes no difference to our argument because we consider only absolute values of the I_js.) But

$$\begin{aligned}
|I_1| &\le \frac{1}{2\lambda}\int_0^r |f(-\lambda - \mathrm{i}y)|\mathrm{e}^{-\pi m y/\lambda}\,\mathrm{d}y \le \frac{\rho}{2\pi m},\\
|I_2| &\le \frac{1}{2\lambda}\int_{-\lambda}^{\lambda} |f(x - \mathrm{i}r)|\mathrm{e}^{-\pi m y/\lambda}\,\mathrm{d}x \le \sigma\mathrm{e}^{-\pi m r/\lambda},\\
|I_3| &\le \frac{1}{2\lambda}\int_0^r |f(\lambda - \mathrm{i}y)|\mathrm{e}^{-\pi m y/\lambda}\,\mathrm{d}y \le \frac{\rho}{2\pi m}.
\end{aligned}$$

Adding the above yields (2.4).

For $m \le -1$ we repeat the exercise except that we swap the Γ_j^+s for Γ_j^-s. □

We define

$$\check{f}_m^{\lambda} = \frac{1}{2\lambda}\int_{-\infty}^{\infty} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x, \qquad m \in \mathbb{Z}$$

– in other words the range of integration is extended to the entire real line.

Lemma 3 *Suppose that $f(z) = \mathrm{e}^{-\alpha z^2}g(z)$, where $\alpha > 0$ and g is entire and uniformly bounded in $(-\infty,\infty)$. Set*

$$c_n = \max_{z\in\tilde{\mathcal{S}}_{r_n}} |g(z)|, \qquad r_n = \frac{\pi|n|}{\lambda\alpha},$$

where $\tilde{\mathcal{S}}_r = \{z \in \mathbb{C} \,:\, |\mathrm{Im}\, z| \le r\}$. Then

$$|\check{f}_m^{\lambda}| \le \frac{\pi^{1/2}c_n}{2\alpha^{1/2}\lambda}\exp\left(-\frac{\pi^2 m^2}{4\lambda^2\alpha}\right), \qquad |m| \le n \tag{2.5}$$

and the decay of Fourier coefficients in this range is super-exponential.

Proof We have

$$\begin{aligned}
\check{f}_m^{\lambda} &= \frac{1}{2\lambda}\int_{-\infty}^{\infty} g(x)\exp\left(-\alpha x^2 - \frac{\pi\mathrm{i}mx}{\lambda}\right)\mathrm{d}x\\
&= \frac{\exp\left(-\frac{\pi^2 m^2}{4\alpha\lambda^2}\right)}{2\lambda}\int_{-\infty}^{\infty} g(x)\exp\left(-\left(\alpha^{1/2}x + \frac{\pi\mathrm{i}m}{2\alpha^{1/2}\lambda}\right)^2\right)\mathrm{d}x\\
&= \frac{1}{2\alpha^{1/2}\lambda}\exp\left(-\frac{\pi^2 m^2}{4\alpha\lambda^2}\right)\int_{-\infty}^{\infty} g\left(\frac{x}{\alpha^{1/2}} - \frac{\pi\mathrm{i}m}{2\alpha\lambda}\right)\mathrm{e}^{-x^2}\,\mathrm{d}x.
\end{aligned}$$

Consequently,

$$|\check{f}^\lambda_m| \le \frac{c_m}{2\alpha^{1/2}\lambda} \exp\left(-\frac{\pi^2 m^2}{4\alpha\lambda^2}\right) \int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x = \frac{\pi^{1/2} c_m}{2\alpha^{1/2}\lambda} \exp\left(-\frac{\pi^2 m^2}{4\alpha\lambda^2}\right)$$

and (2.5) follows because $c_m = c_{|m|}$ and the c_ms form a monotonically increasing sequence for $m \ge 0$. □

Corollary 1 *Suppose that instead of being entire, g is analytic in the closed upper half plane $\{z \in \mathbb{C} : \operatorname{Im} z \ge 0\}$. Then (2.5) holds for $-n \le m \le 0$. By the same token, if g is analytic in the closed lower half plane, (2.5) is valid for $0 \le m \le n$.*

The proof of the corollary is a direct consequence of the proof of Lemma 3. Note that similar result is applicable to Lemma 2, with identical proof.

Lemma 4 *Suppose that $f(z) = \mathrm{e}^{-\alpha z^2} g(z)$, where $\alpha > 0$ and g is entire. Then, for every $n \ge 1$ it is true that*

$$|\hat{f}^\lambda_m| \le \frac{\pi^{1/2} c_n}{2\alpha^{1/2}\lambda} \exp\left(-\frac{\pi^2 m^2}{4\alpha\lambda^2}\right) + \frac{c_0}{\pi^{1/2}\alpha\lambda^2}\mathrm{e}^{-\alpha\lambda^2}, \qquad |m| \le n. \tag{2.6}$$

Proof We have

$$\hat{f}^\lambda_m = \check{f}^\lambda_m - \frac{1}{2\lambda}\int_{-\infty}^{-\lambda} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x - \frac{1}{2\lambda}\int_{\lambda}^{\infty} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x.$$

However,

$$\left|\int_{\lambda}^{\infty} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x\right| \le c_0 \int_{\lambda}^{\infty} \mathrm{e}^{-\alpha x^2}\,\mathrm{d}x = \frac{c_0}{\alpha^{1/2}} \int_{\alpha^{1/2}\lambda}^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x.$$

Since

$$\int_t^{\infty} \mathrm{e}^{-x^2}\,\mathrm{d}x \le \frac{\mathrm{e}^{-t^2}}{\pi^{1/2}(1+t)}, \qquad t \ge 0,$$

(DLMF 2016, 7.8.3), we deduce that

$$\left|\int_{\lambda}^{\infty} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x\right| \le \frac{c_0}{\pi^{1/2}\alpha^{1/2}} \cdot \frac{\mathrm{e}^{-\alpha\lambda^2}}{1+\alpha^{1/2}\lambda} \le \frac{c_0}{\pi^{1/2}\alpha\lambda}\mathrm{e}^{-\alpha\lambda^2}.$$

Since an identical bound applies to $\left|\int_{-\infty}^{-\lambda} f(x)\mathrm{e}^{-\pi\mathrm{i}mx/\lambda}\,\mathrm{d}x\right|$, (2.6) follows upon division by 2λ. □

In line with Corollary 1, (2.6) holds for $0 \le m \le n$ if g is analytic for $\operatorname{Im} z \le 0$ and for $-n \le m \le 0$ if analyticity occurs for $\operatorname{Im} z \ge 0$. This is illustrated by the the third graph in Fig. 2.1. Since $g(z) = (1+\mathrm{i}x)^{-1}$ has a pole at $+\mathrm{i}$ but is analytic in the lower half plane, its positive coefficients display super-exponential decay, while negative coefficients, governed by Lemma 2, decay exponentially – in both cases, until they hit the 'floor'.

Compare (2.3), (2.4) and (2.6). In each case, in the relevant range $m_0 \le |m| \le n$, we have

$$|\hat{f}_m^\lambda| \le p_{n,m} + q_n \mathrm{e}^{-\tau_{n,m}}, \tag{2.7}$$

where p_n is very small, while $\tau_{n,m} > 0$ and the $\tau_{n,m}$s form a monotonically increasing (in $|m|$) sequence: specifically

1. $f \in \mathrm{C}^N[-\lambda, \lambda]$: $m_0 = \lceil \frac{\lambda}{\pi} \rceil$,

$$p_{n,m} = \frac{1 - \left(\frac{\lambda}{\pi m}\right)^N}{2(\pi m - \lambda)} \max_{j=0,\ldots,N-1} |f^{(j)}(\pm\lambda)|, \quad q_n \equiv \|f^{(N)}\|_\infty, \quad \tau_{n,m} = -N \log \frac{\lambda}{\pi m};$$

2. f analytic in $|\mathrm{Re}\, z| \le \lambda$, $|\mathrm{Im}\, z| \le r$: $m_0 = 1$ and

$$p_{n,m} = \frac{\max_{|y|\le r} |f(\pm\lambda + \mathrm{i}y)|}{\pi |m|}, \quad q_n = \max_{|x|\le\lambda} |f(x \pm \mathrm{i}r)|, \quad \tau_{n,m} = \frac{\pi r m}{\lambda};$$

3. f entire, $f(z) = \mathrm{e}^{-\alpha z^2} g(z)$ with $\alpha > 0$: $m_0 = 0$ and

$$p_{n,m} = \frac{c_0 \mathrm{e}^{-\alpha\lambda^2}}{\pi^{1/2}\alpha\lambda^2}, \qquad q_n = \frac{\pi^{1/2} c_n}{2\alpha^{1/2}\lambda}, \qquad \tau_{n,m} = \frac{\pi^2 m^2}{4\alpha\lambda^2}.$$

2.2 Choosing a good λ

How to choose a good λ? Fig. 2.2 displays the size of stretched Fourier coefficients for the same wave packet $\mathrm{e}^{-x^2/2}\sin(30x)$ and three values of λ. Evidently, two processes are in competition:

- The smaller λ, the faster the convergence; but
- The larger λ, spectral rate of decay persists for longer.

Therefore we need to choose λ large enough to ensure that rapid decay of coefficients takes place in the entire range of desired accuracy – but not much larger!

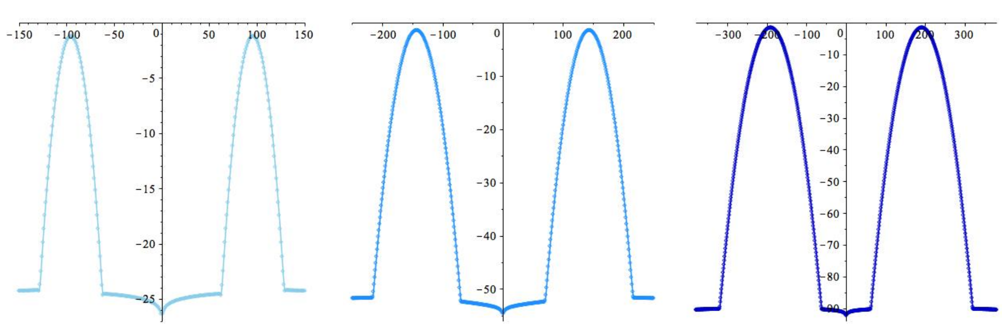

Figure 2.2: $\log_{10} |\hat{f}_m^\lambda|$ for the wave packet $f(x) = \mathrm{e}^{-x^2/2}\sin(30x)$ and $\lambda = 10, 15, 20$.

Good choice of λ depends on f, yet we wish, using the previous subsection, to reduce this dependence to few essential features of f – essentially, its rate of decay for $|x| \gg 1$ and its smoothness. For example, if $f(z) = g(z)\mathrm{e}^{-\alpha z^2}$, where $\alpha > 0$ and g is entire, it follows from our analysis that we need to render $\mathrm{e}^{-\alpha\lambda^2}/(\alpha\lambda^2)$ sufficiently small. But

$$\frac{\mathrm{e}^{-\alpha\lambda^2}}{\alpha\lambda^2} = \varepsilon \qquad \Rightarrow \qquad \alpha\lambda^2\mathrm{e}^{\alpha\lambda^2} = \frac{1}{\varepsilon} \qquad \Rightarrow \qquad \alpha\lambda^2 = \mathrm{W}(\varepsilon^{-1}),$$

where W is the *Lambert W-function* (DLMF 2016, 4.13.1), the principal branch of the inverse function of $\mathrm{W}\mathrm{e}^{\mathrm{W}} = x$. We deduce that a good choice of λ is

$$\lambda = \left[\frac{\mathrm{W}(\varepsilon^{-1})}{\alpha}\right]^{1/2}. \tag{2.8}$$

Following the same logic, once f is analytic in $|\mathrm{Im}\, z| \le r$, we might choose λ as the least positive solution of the equation

$$\max_{|y|\le r} |f(\pm\lambda + \mathrm{i}y)| = \varepsilon. \tag{2.9}$$

Unless $|f|$ grows very rapidly for $|\pm\lambda+\mathrm{i}y|$, it is sufficient (and far easier) to let λ be the least positive solution of $\max\{|f(-\lambda)|, |f(\lambda)|\} = \varepsilon$. Finally, if $f \in \mathrm{C}^N(\mathbb{R})$ (inclusive of the case $f \in \mathrm{C}^\infty(\mathbb{R})$), we may choose λ as the least positive solution of the equation

$$\max_{j=0,\ldots,N-1} |f^{(j)}(\pm\lambda)| = \varepsilon \tag{2.10}$$

– if $N = \infty$ we restrict the range of j in (2.10) to a finite set.

The choices (2.8)–(2.10) are not optimal and typically λ is marginally too large. Yet, they represent a good rule of a thumb in the implementation of our approach.

Our results help not just in identifying a good λ but also restricting *a priori* the range of $m \in \mathbb{Z}$ such that $|\hat{f}_m^\lambda| > \varepsilon$ – these are the only values which need be used in our computations. Once a function is analytic in $\mathcal{S}_r$, (2.4) implies that we need ms so that roughly $\exp(-\pi r|m|/\lambda) > \varepsilon$, i.e.

$$|m| < \frac{-\lambda \log \varepsilon}{\pi r}. \tag{2.11}$$

By the same token, for $f(x) = \mathrm{e}^{-\alpha x^2} g(x)$ with an entire g, it follows from (2.6) that a good range of ms is such that $\exp\left(-\frac{\pi^2 m^2}{4\lambda^2\alpha}\right) > \varepsilon$, hence

$$|m| < \frac{2\lambda}{\pi} \left[-\alpha \log \varepsilon\right]^{1/2}. \tag{2.12}$$

In practice it is always safe to err on the side of caution and take slightly larger range of ms. Moreover, whether we are using (2.11) or (2.12), once using FFT to compute Fourier coefficients we might need to round up the range to the nearest power of 2.

To illustrate our narrative, we have computed stretched Fourier expansions of six functions, in each case imposing $\varepsilon = 10^{-20}$ and choosing λ accordingly:

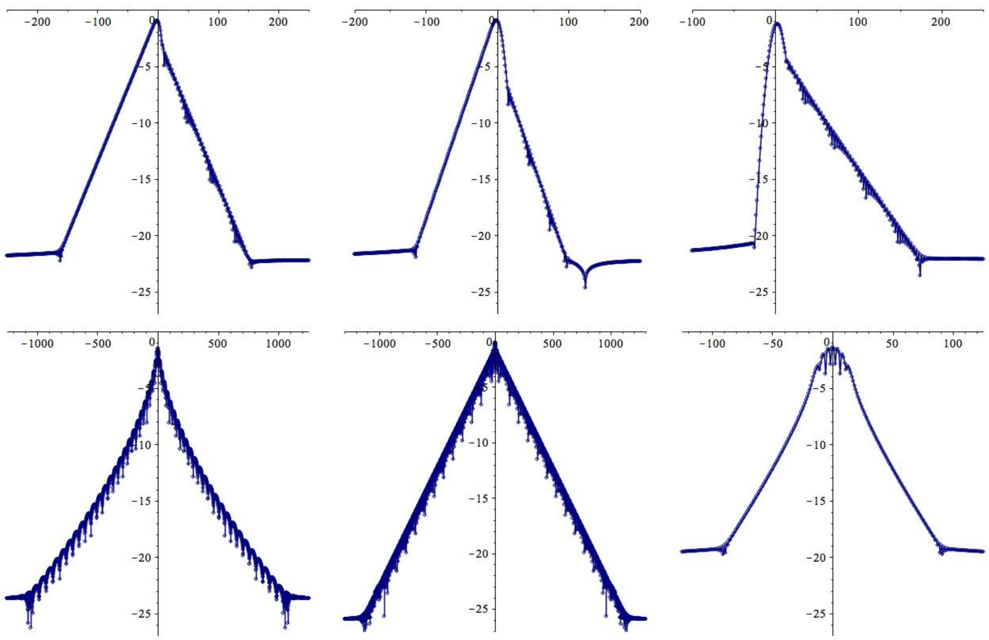

Figure 2.3: The decay of coefficients, drawn in $\log_{10}$ scale, for the six examples.

1. $f(x) = \frac{e^{-x^2/2}}{1+i\sin x}$, a meromorphic function with poles at $-i\log(\sqrt{2}-1)+2\pi k$, $k \in \mathbb{Z}$, $\lambda = \left[2W(10^{20})\right]^{1/2} \approx 9.1986$;

2. $f(x) = \frac{e^{-x^2}}{1+i\sin x}$, similar to the previous example except with much more rapid decay, $\lambda = \left[W(10^{20})\right]^{1/2} \approx 6.5044$;

3. $f(x) = e^{-x^2/2}\log(1+\frac{1}{2}e^{ix})$, analytic for $\operatorname{Im} z > -\log 2$ and with branch cuts at $\pi(2k+1)+iy$, $y < -\log 2$, $k \in \mathbb{Z}$, again $\lambda \approx 9.1986$;

4. $f(x) = \exp\left(-\frac{x^2}{2} - \frac{1}{x^2}\right)$, a $C^\infty(\mathbb{R})$ function. λ as before;

5. $f(x) = \frac{1}{1+x^{20}}$, a meromorphic function which tends fast, yet sub-exponentially to zero for $|x| \gg 1$, with λ as the zero of $\frac{1}{1+\lambda^{20}} = 10^{-20}$, $\lambda \approx 10.0000$;

6. The $C^5(\mathbb{R})$ function

$$f(x) = \operatorname{sgn}(x)\, e^{-x^2/2}\left[\frac{1-6x^2+x^4}{2}\log(1+x^2)+\frac{7}{2}x^2-\frac{25}{12}x^4-4x(1-x)\arctan x\right],$$

$\lambda = [-2\log 10^{-20}]^{1/2} \approx 9.5971$.

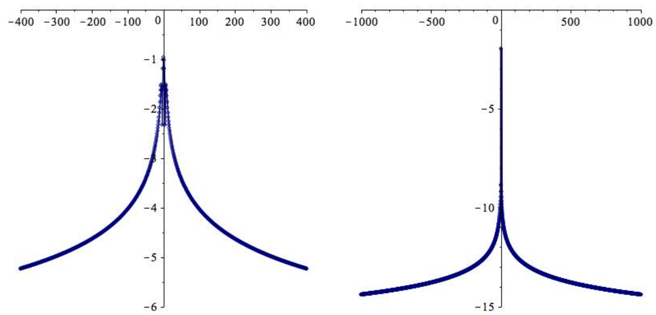

Figure 2.4: The decay of coefficients, drawn in $\log_{10}$ scale, for further, slowly-convergent two examples.

Our first observation is that our choice of λ is often (but not always!) fairly conservative and the 'floor' is typically lower than at -20. The rate of decay is typically exponential (corresponding to a straight line in the figure) because most functions are meromorphic, except that the third function is analytic in a half plane, while the fourth function, which is C^∞, decays slower than exponentially (yet faster than the reciprocal of any polynomial).

Needless to say, once f is not C^N or fails to decay sufficiently fast for $|x| \gg 1$, the entire construction is bound to collapse. Thus, in Fig. 2.4 on the left we have computed the size of the Fourier coefficients for $f(x) = |x|\mathrm{e}^{-x^2/2}$ with $\lambda \approx 9.1986$. Although the function decays very rapidly, the singularity at the origin is sufficient to slow down Fourier coefficients to linear decay: we hit the 'floor' from the very beginning. In other instances, while the function exhibits all the right smoothness, its slow rate of decay means that the least value of λ is not realistic. In Fig. 2.4 on the right we display the size of the coefficients for $f(x) = 1/(1 + x^4)$ and the arbitrarily-chosen $\lambda = 100$: the decay is linear. To obtain the 'sombrero effect' we would need, using our approach, to take $\lambda \approx 10^5$ (for $\varepsilon = 10^{-20}$) which is completely impractical.

3 Connection coefficients and Hermite expansions

Let $\boldsymbol{P} = \{p_m\}_{m\ge 0}$ and $\boldsymbol{Q} = \{q_m\}_{m\ge 0}$ be two polynomial bases such that $\deg p_m = \deg q_m = m$. Then there exist numbers $a_{k,m}$, $0 \le k \le m$, such that

$$q_m(x) = \sum_{k=0}^{m} a_{m,k} p_m(x), \qquad k = 0, \ldots, m \quad n \ge 0. \tag{3.1}$$

These numbers are called *connection coefficients* of the two polynomial sequences (Ismail 2005). (This should not be confused with connection coefficients in the context of differential geometry and Riemannian manifolds (Abraham & Marsden 1978).) For example

$$\mathrm{P}_m(x) = \frac{1}{2^{2m-1}} \sum_{k=0}^{\lfloor m/2 \rfloor} \binom{2k}{k}\binom{2m-2k}{m-k} \mathrm{T}_{m-2k}(x),$$

where, for even m, the coefficient for $k = m/2$ need be halved. Connection coefficients allow us to convert an expansion in $\boldsymbol{P}$ into an expansion in $\boldsymbol{Q}$ for $m = 0, \ldots, n$ at the cost of $\mathcal{O}(n^2)$ operations – less if the coefficients $a_{m,k}$ decay rapidly for growing k and we wish to evaluate the new expansion to given accuracy.

In our case we wish to re-express a Fourier expansion in $[-\lambda, \lambda]$ into an expansion in either Hermite polynomials or Hermite functions. Neither Fourier coefficients nor Hermite functions are polynomials yet all we need is to allow the sum in (3.1) be over all integers, hoping that the coefficients decay sufficiently rapidly to allow for truncation. Thus,

$$\mathrm{e}^{\mathrm{i}\pi kx/\lambda} = \sum_{m=0}^{\infty} a_{k,m}^{\mathsf{P}} \mathrm{H}_m(x) = \sum_{m=0}^{\infty} a_{k,m}^{\mathsf{F}} \psi_m(x), \qquad k \in \mathbb{Z}.$$

Recalling the Fourier expansion of (sufficiently smooth) f in the window $[-\lambda, \lambda]$,

$$f(x) = \sum_{k=-\infty}^{\infty} \hat{f}_k^{\lambda} \exp\left(\frac{\mathrm{i}\pi kx}{\lambda}\right),$$

we denote the corresponding expansions in Hermite polynomials and functions by

$$f(x) = \sum_{m=0}^{\infty} \hat{f}_m^{\mathsf{P}} \mathrm{H}_m(x) \qquad \text{and} \qquad f(x) = \sum_{m=0}^{\infty} \hat{f}_m^{\mathsf{F}} \psi_m(x)$$

respectively and note that (subject to very mild conditions on f, allowing interchange of infinite sums)

$$\hat{f}_m^{\mathsf{P}} = \sum_{k=-\infty}^{\infty} \hat{f}_k^{\lambda} a_{k,m}^{\mathsf{P}}, \quad \hat{f}_m^{\mathsf{F}} = \sum_{k=-\infty}^{\infty} \hat{f}_k^{\lambda} a_{k,m}^{\mathsf{F}}, \qquad m \geq 0. \tag{3.2}$$

The analysis in the sequel can be unified by letting $\Psi_m^{(\beta)}(x) = \mathrm{e}^{-\beta x^2} \mathrm{H}_m(x)$, $\beta \in [0, \frac{1}{2}]$, and seeking an expansion in the orthogonal basis $\{\Psi_n^{(\beta)}\}_{n \geq 0}$ with respect to the inner product $\langle f, g \rangle = \int_{-\infty}^{\infty} f(x) g(x) \mathrm{e}^{-(1-2\beta)x^2}\, \mathrm{d}x$: Hermite polynomials and functions correspond to $\beta = 0$ and $\beta = \frac{1}{2}$ respectively. However, it is probably clearer to distinguish the two cases.

Here we used the analytic extension of the basis functions $\mathrm{e}^{\mathrm{i}\pi kx/\lambda}$ of the stretched Fourier expansion over $[-\lambda, \lambda]$ to the real line, which amounts to a periodic modification of the original function. However, the Hermite polynomials together with their weight and the Hermite functions are rapidly decaying, so that for the typical ranges of λ and Hermite indices $m = 0, \ldots, n$ this effect is negligible.

If this assumption fails, one can e.g. use the extension $\mathrm{e}^{\mathrm{i}\pi kx/\lambda} 1_{[-\lambda,\lambda]}$, where the recurrence relations (3.4) and (3.7) can be derived from the three-term recurrence relation of the Hermite polynomials. However, in our setting it complicates the analysis without any additional benefit.

3.1 Hermite polynomials

Lemma 5 *For every $m \ge 0$ and $k \in \mathbb{Z}$ it is true that*

$$a^{\mathsf{P}}_{k,m} = \frac{1}{m!}\left(\frac{\mathrm{i}\pi k}{2\lambda}\right)^m \exp\left(-\left(\frac{\pi k}{2\lambda}\right)^2\right). \tag{3.3}$$

Proof Substituting the Fourier expansion and interchanging integration and summation for sufficiently smooth f,

$$\begin{aligned}\hat{f}^{\mathsf{P}}_m &= \frac{\pi^{-1/2}}{2^m m!}\int_{-\infty}^{\infty} f(x)\mathrm{H}_m(x)\mathrm{e}^{-x^2}\,\mathrm{d}x = \frac{\pi^{-1/2}}{2^m m!}\int_{-\infty}^{\infty}\left(\sum_{k=-\infty}^{\infty}\hat{f}^{\lambda}_k \mathrm{e}^{\mathrm{i}\pi k x/\lambda}\right)\mathrm{H}_m(x)\mathrm{e}^{-x^2}\,\mathrm{d}x\\ &= \frac{1}{2^m m!\pi^{1/2}}\sum_{k=-\infty}^{\infty}\hat{f}^{\lambda}_k\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2}\mathrm{H}_m(x)\,\mathrm{d}x,\end{aligned}$$

therefore

$$a^{\mathsf{P}}_{k,m} = \frac{1}{2^m m!\pi^{1/2}}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2}\mathrm{H}_m(x)\,\mathrm{d}x, \qquad m \in \mathbb{Z}, \quad m \ge 0.$$

We next form the generating function

$$\mathcal{A}_k(t) := \sum_{m=0}^{\infty} a^{\mathsf{P}}_{k,m} t^m = \frac{1}{\pi^{1/2}}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2}\sum_{m=0}^{\infty}\frac{\mathrm{H}_m(x)}{m!}\left(\frac{t}{2}\right)^m\,\mathrm{d}x.$$

A generating function for Hermite polynomials is

$$\sum_{m=0}^{\infty}\frac{H_m(x)}{m!}t^m = \mathrm{e}^{2xt - t^2}$$

(DLMF 2016, 18.12.15), therefore, changing variables as appropriate,

$$\begin{aligned}\mathcal{A}_k(t) &= \frac{1}{\pi^{1/2}}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2}\mathrm{e}^{xt - t^2/4}\,\mathrm{d}x\\ &= \pi^{-1/2}\exp\left(\frac{\mathrm{i}\pi k t}{2\lambda} - \frac{\pi^2 k^2}{4\lambda^2}\right)\int_{-\infty}^{\infty}\exp\left(-\left(x - \frac{t}{2} - \frac{\pi \mathrm{i} k}{2\lambda}\right)^2\right)\,\mathrm{d}x\\ &= \pi^{-1/2}\exp\left(\frac{\mathrm{i}\pi k t}{2\lambda} - \frac{\pi^2 k^2}{4\lambda^2}\right)\int_{-\infty}^{\infty}\mathrm{e}^{-x^2}\,\mathrm{d}x = \exp\left(\frac{\mathrm{i}\pi k t}{2\lambda} - \frac{\pi^2 k^2}{4\lambda^2}\right).\end{aligned}$$

Therefore

$$a^{\mathsf{P}}_{k,m} = \frac{1}{m!}\frac{\partial^m \mathcal{A}_k(t)}{\partial t^m}\Big|_{t=0} = \frac{1}{m!}\left(\frac{\mathrm{i}\pi k}{2\lambda}\right)^m \exp\left(-\frac{\pi^2 k^2}{4\lambda^2}\right)$$

and the lemma is true. □

Note that $a^{\mathsf{P}}_{k,0} = \exp\big(-\pi^2 k^2/(4\lambda^2)\big)$ and

$$a^{\mathsf{P}}_{k,m+1} = \frac{\mathrm{i}\pi k}{2\lambda(m+1)}a^{\mathsf{P}}_{k,m}, \qquad m, k \ge 0, \tag{3.4}$$

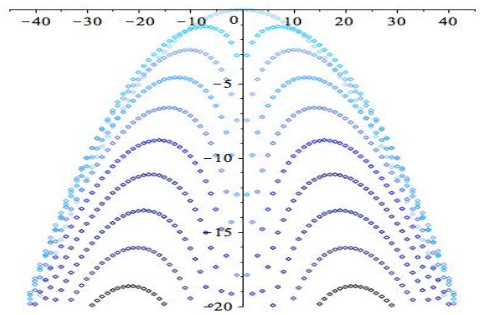

Figure 3.1: $\log_{10}|a^{\mathsf{P}}_{k,m}|$ for $m = 0, 3, 6, \ldots, 27$ (darker shade denotes larger m) and $\lambda = 9.1986$.

allowing for rapid calculation of the coefficients.

The coefficients $a^{\mathsf{P}}_{k,m}$ decay very rapidly. Their magnitude is displayed in logarithmic scale in Fig. 3.1 and it is evident that, for any stipulated accuracy, just a finite (and fairly small) number of coefficients need be calculated: the larger λ, the more coefficients.

For a specific coefficient $\hat{f}^{\mathsf{P}}_m$ we fix m and form the sum over k. Looking at Fig. 3.1 shows that only few terms are relevant. Treating $k > 0$ as a continuous variable, we find that

$$\frac{\mathrm{d}^2 \log |a^{\mathsf{P}}_{km}|}{\mathrm{d}k^2} = -\frac{m}{k^2} - \frac{\pi}{2\lambda^2} \leq -\frac{\pi^2}{2\lambda^2},$$

which shows strict uniform concavity. Hence for any prescribed precision ε there are only finitely many indices not satisfying $|a_{k,m}| \leq \epsilon |a_{K,m}|$ where $|a_{K,m}|$ is the largest coefficient. Moreover, the number of relevant coefficients is bounded uniformly in m. To find the relevant coefficients let

$$h_m(x) = \frac{y^m}{m!} \mathrm{e}^{-y^2},$$

therefore $a^{\mathsf{P}}_{k,m} = h_m(\pi k/(2\lambda))$. The function h_m has maxima at $\pm y_m = \pm(m/2)^{1/2}$ and, using twice the Stirling formula,

$$h_m(\pm y_m) = \frac{1}{m!}\left(\frac{m}{2}\right)^{m/2} \mathrm{e}^{-m/2} \approx \frac{1}{2^{m+1/2}\Gamma\left(\frac{m}{2}+1\right)}$$

decreases very rapidly as a function of m. The maximal value of h_m helps us to choose the range of ms necessary to 'intercept' all $|a^{\mathsf{P}}_{k,m}| > \varepsilon$: the rule of the thumb is to choose $0 \leq m \leq m^\star$ such that $h_{m^\star}(y_{m^\star}) \approx \varepsilon$. Computer experimentation demonstrates that an almost perfect fit is

$$m^\star(\varepsilon) \approx \left(0.7321 + 1.4174 \log \frac{1}{\varepsilon}\right)^{4/5}. \tag{3.5}$$

3.2 Hermite functions

The derivation of the coefficients $a^{\mathsf{F}}_{k,m}$ is similar to their polynomial counterparts but it is convenient first to compute

$$\tilde{a}^{\mathsf{F}}_{k,m} = \frac{1}{2^m m! \pi^{1/2}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\pi m x/\lambda - x^2/2} \mathrm{H}_m(x)\,\mathrm{d}x$$

and subsequently let

$$a^{\mathsf{F}}_{k,m} = (-1)^m (2^m m!)^{1/2} \pi^{1/4} \tilde{a}^{\mathsf{F}}_{k,m}.$$

Lemma 6 *For every $m \geq 0$ and $k \in \mathbb{Z}$ it is true that*

$$a^{\mathsf{F}}_{k,m} = \frac{\mathrm{i}^m \pi^{1/4}}{2^{(m-1)/2}(m!)^{1/2}} \mathrm{H}_m\left(\frac{\pi k}{\lambda}\right) \exp\left(-\frac{\pi^2 k^2}{2\lambda^2}\right). \tag{3.6}$$

Proof Let

$$\mathcal{B}_k(t) := \sum_{m=0}^{\infty} \tilde{a}^{\mathsf{F}}_{k,m} t^m = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2/2} \sum_{m=0}^{\infty} \frac{\mathrm{H}_m(x)}{m!} \left(\frac{t}{2}\right)^m \mathrm{d}x.$$

Using twice a generating function for Hermite polynomials,

$$\begin{aligned}
\mathcal{B}_k(t) &= \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\pi k x/\lambda - x^2/2} \mathrm{e}^{xt - t^2/4}\,\mathrm{d}x = \frac{\mathrm{e}^{t^2/4}}{\pi^{1/2}} \int_{-\infty}^{\infty} \exp\left(\frac{\mathrm{i}\pi k(x+t)}{\lambda} - \frac{1}{2}x^2\right)\mathrm{d}x \\
&= 2^{1/2} \exp\left(-\frac{\pi^2 k^2}{2\lambda^2} + \frac{\mathrm{i}\pi k t}{\lambda} + \frac{1}{4}t^2\right) \\
&= 2^{1/2} \exp\left(-\frac{\pi^2 k^2}{2\lambda^2}\right) \exp\left(2\left(\frac{\pi k}{\lambda}\right)\left(\frac{\mathrm{i}t}{2}\right) - \left(\frac{\mathrm{i}t}{2}\right)^2\right) \\
&= 2^{1/2} \exp\left(-\frac{\pi^2 k^2}{2\lambda^2}\right) \sum_{m=0}^{\infty} \frac{1}{m!} \mathrm{H}_m\left(\frac{\pi k}{\lambda}\right)\left(\frac{\mathrm{i}t}{2}\right)^m
\end{aligned}$$

and (3.6) follows. □

Applying the three-term recurrence relation

$$\mathrm{H}_{m+1}(x) = 2x\mathrm{H}_m(x) - 2m\mathrm{H}_{m-1}(x)$$

(DLMF 2016, 18.9) to (3.6) we obtain a rapid method for the evaluation of the $a^{\mathsf{F}}_{m,k}$s, namely

$$a^{\mathsf{F}}_{m+1,k} = \frac{\mathrm{i}\pi k}{(2m+2)^{1/2}\lambda} a^{\mathsf{F}}_{k,m} + \left(\frac{m}{m+1}\right)^{1/2} a^{\mathsf{F}}_{k,m-1}, \tag{3.7}$$

a counterpart of (3.4). Unfortunately, the $a^{\mathsf{F}}_{k,m}$s decay very slowly indeed (a counterpart of Fig. 3.1 would have been of little use), yet according to a pattern, displayed in Fig. 3.2. Essentially, until $|k|$ becomes fairly large, $|a^{\mathsf{F}}_{k,m}| = \mathcal{O}(1)$, while oscillating rapidly. Only when $|k| \gg 1$ the coefficients decrease very fast indeed.

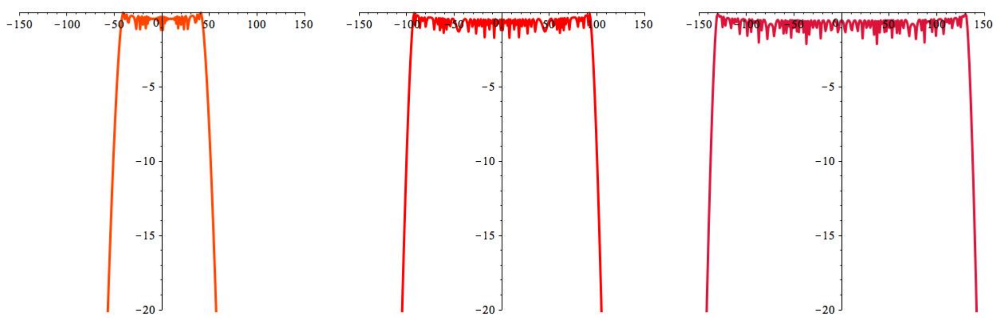

Figure 3.2: $\log_{10}|a^{\mathsf{F}}_{m,k}|$ for $\lambda \approx 9.1985$ and (from left) $m = 100, 500$ and 1000.

To look further into the behaviour of the $a^{\mathsf{F}}_{k,m}$s for large m and fixed k, we employ the asymptotic formula

$$\mathrm{H}_m(y) \sim \frac{(2\lfloor (m+1)/2\rfloor)!}{(\lfloor (m+1)/2\rfloor)!} \mathrm{e}^{y^2/2} \cos\left((2m+1)^{1/2} y - \frac{\pi m}{2}\right), \qquad m \gg 1$$

(DLMF 2016, 18.15.27). Using the Stirling formula we deduce from (3.7) after tedious, yet simple algebra that

$$|a^{\mathsf{F}}_{k,m}| \sim \frac{2}{m^{1/4}} \cos\left(\frac{\pi(2m+1)^{1/2}k}{\lambda} - \frac{\pi m}{2}\right), \qquad m \gg 1.$$

On the other hand, for fixed m and large $|k|$ we exploit $H_m(x) \approx (2x)^m$, $|x| \gg 1$, to argue that

$$|a^{\mathsf{F}}_{k,m}| \approx \frac{\pi^{1/4} 2^{(m+1)/2}}{(m!)^{1/2}} \left(\frac{k\pi}{\lambda}\right)^m \exp\left(-\frac{\pi^2 k^2}{2\lambda^2}\right) \qquad |k| \gg 1,$$

and this becomes very small for large $|k|$ because the exponential term always wins.

We should not be surprised by the clearly inferior behaviour of the $a^{\mathsf{F}}_{k,m}$s in comparison to the $a^{\mathsf{P}}_{k,m}$s. The latter might well be much smaller but they multiply Hermite polynomials, which rapidly become very large, while Hermite function coefficients always multiply the uniformly bounded ψ_ms.

3.3 Attenuated connection coefficients

The conclusion to the last two subsections is, on the face of it, disappointing. The connection coefficients of Hermite polynomials decay rapidly, yet the polynomials themselves grow, while the connection coefficients of the uniformly-bounded Hermite functions stubbornly resist getting small as m increases – if at all, they are $\mathcal{O}(1)$ for an increasing range of ks. The entire idea of first deriving the $\hat{f}^{\lambda}_k$s by FFT and then using (3.2) to produce Hermite coefficients clearly appears to be the wrong approach.

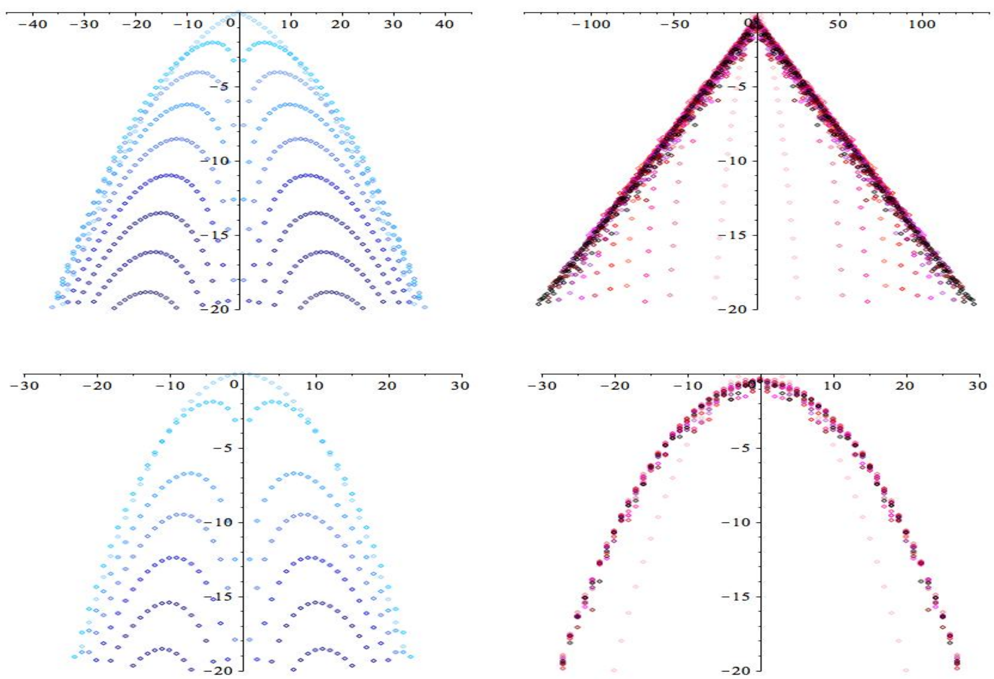

Figure 3.3: Attenuated connection coefficients, all with $\lambda = 9.1986$: on the left the $\log_{10}|\check{a}^{\mathsf{P}}_{k,m}|$ for $m = 0, 3, 6, \ldots, 27$ and on the left $\log_{10}|\check{a}^{\mathsf{F}}_{k,m}|$ for $m = 0, 100, 200, \ldots, 1000$. Darker shade denotes larger m. In the top row we attenuate by $\exp\!\left(-\frac{\pi r|k|}{\lambda}\right)$, $r = 1$, and in the bottom row by $\exp\!\left(-\frac{\pi^2 k^2}{4\alpha\lambda^2}\right)$, $\alpha = \frac{1}{2}$.

But is it? In the analysis of Subsections 3.1–2 we have disregarded the fact that Fourier coefficients $\hat{f}^{\lambda}_m$ themselves decay rapidly. For example, once f is analytic in the strip $|\mathrm{Im}\, z| \le r$, we know from (2.4) that within the 'sombrero range' (hence disregarding the negligible 'floor') $|\hat{f}^{\lambda}_k| \le c\exp\!\left(-\frac{\pi r}{\lambda}|k|\right)$. Therefore the truncation rule is to stop once

$$\exp\!\left(-\frac{\pi r}{\lambda}|k|\right)|a^{\mathsf{X}}_{k,m}| < \varepsilon,$$

where X is either P or F. Likewise, if f is entire then (2.6) implies that $|\hat{f}^{\lambda}_k| \le c\exp\!\left(-\frac{\pi^2 k^2}{4\alpha\lambda^2}\right)$, hence the termination rule is $\exp\!\left(-\frac{\pi^2 k^2}{4\alpha\lambda^2}\right)|a^{\mathsf{X}}_{k,m}| < \varepsilon$.

Denoting attenuated connection coefficients by $\check{a}^{\mathsf{X}}_{k,m}$, where $\mathsf{X} \in \{\mathsf{P}, \mathsf{F}\}$, Fig. 3.3 displays their size for these two different attenuation procedures. It is clear that, employing this extra information on the rate of decay of Fourier coefficients reduces drastically the number of connection constants that need be computed in an implementation of (3.2). In the case of Hermite polynomials the uniform concavity is preserved and typically even more terms can be discarded, while for Hermite functions this makes all the difference between an infeasible algorithm and one which, although not very fast, is at least implementable.

3.4 Toward a Hermite solver

The road leading from expressions (3.3) and (3.6) to an algorithm for the computation of $\hat{f}_m^{\mathsf{X}}$, $m = 0, \ldots, n$, to given accuracy $\varepsilon > 0$ is clear. First we need to compute a stretched Fourier expansion by FFT with $2M$ points for a sufficiently large M. The choice of M is governed by whether we want an Hermite polynomial or functional expansion (M should be much larger for an expansion in Hermite functions), by the nature of the function f (its smoothness and its rate of decay for $|x| \gg 1$) and, of course, M needs to be a highly composite integer to allow for the use of FFT. Altogether, this step costs $\mathcal{O}(M \log_2 M)$ operations.

Once $\hat{f}_k^{\lambda}$, $-M+1 \le k \le M$, are available, we compute the connection coefficients $a_{k,m}^{\mathsf{X}}$, using either (3.4) or (3.7), for k in the above range and $m = 0, \ldots, n$. Note that we do not need all these coefficients, as is clear from Fig. 3.3, just the coefficients for which the *attenuated coefficients* (which we never compute but which always exist in the background!) are larger than ε and, upon better understanding of Fig. 3.3, we can reduce the cost. Finally, we compute

$$\hat{f}_m^{\mathsf{P}} \approx \sum_{k=-M+1}^{M} \hat{f}_k^{\lambda} a_{k,m}^{\mathsf{P}} \quad \text{or} \quad \hat{f}_m^{\mathsf{F}} \approx \sum_{k=-M+1}^{M} \hat{f}_k^{\lambda} a_{k,m}^{\mathsf{F}}, \qquad m = 0, \ldots, n$$

at the cost of $\mathcal{O}(Mn)$.

In the case of Hermite polynomials, we can find for a prescribed precision ε a constant K such that only K terms are needed. This reduces the problem to a fast algorithm in $\mathcal{O}(M \log_2 M + Kn)$ operations.

For a sufficiently decaying function f, we can also consider the expansion of $f(x)\mathrm{e}^{x^2}$ into Hermite polynomials as a way to compute the expansion into Hermite functions. In fact, one can use natural intermediate scales with $f(x)\mathrm{e}^{\beta x^2}$, see (Dietert 2016).

Even though this gives a fast algorithm for sufficiently decaying functions, the discussion of the maximum of h_m at the end of section 3.1 shows that we need $\sim M^2$ Hermite coefficients to approximate a function we can approximate with M stretched Fourier coefficients.

4 Conclusions

In this paper we have introduced a simple approach, based on stretched Fourier expansions, to approximate functions on the real line (and, by implication, on $\mathbb{R}^d$ for reasonably small $d \ge 1$). While this approach can be used as a first step toward the computation of an expansion in Hermite functions or Hermite polynomials, there are good reasons to believe that in most settings it is preferable to use stretched Fourier expansions in the first place.

This methodology is particularly powerful in quantum calculations in the semiclassical regime, since the solution is usually a linear combination of wave packets (1.2). While this can be a basis for a numerical method (Faou et al. 2009, Lasser & Troppmann 2014), other methods do not attempt to model the evolution of wave packets explicitly (Bader et al. 2014, Lubich 2008) but wave packets should be always at the back of our mind while solving dispersive equations. In particular, solving such equations with spectral methods, it is a sound policy to represent the underlying solution in a basis which represents well linear combinations of wave packets.

This is the place to mention that a solution of quantum equations (and, in greater generality, dispersive equations) is not simply a linear combination with time-dependent coefficients of the same wave packets. The matrices P and Q and the vector $\boldsymbol{p}$ in (1.2) are time dependent. Moreover, wave packets can form, reform, change amplitude, combine and split: in quantum scattering, for example, a wave packet splits into typically very large number of separate wave packets, each of different amplitude and frequency, scattering in diverse directions. Practical implementation of stretched Fourier basis in this setting is considerably more complicated than just finding the least eigenvalue of $\mathrm{Im}\, PQ^{-1}$ and using it to identify good λ using (2.8).

A simple policy is to confine the solution t any time $t \geq 0$ to a 'window' $[a_-(t), a_+(t)]$ once exponentially-small terms are disregarded: one policy might be to identify $a_\pm(t)$, translate linearly into $[-[a_+(t) - a_-(t)]/2, [a_+(t) - a_-(t)]/2]$ and set $\lambda = [a_+(t) - a_-(t)]/2$. The precise implementation mechanism is a matter for future research, while bearing in mind the competing imperatives of choosing $\lambda = \lambda(t)$ large enough so that all the 'significant action' is confined to $[-\lambda, \lambda]$, yet small enough to ensure more rapid convergence of stretched Fourier expansion.

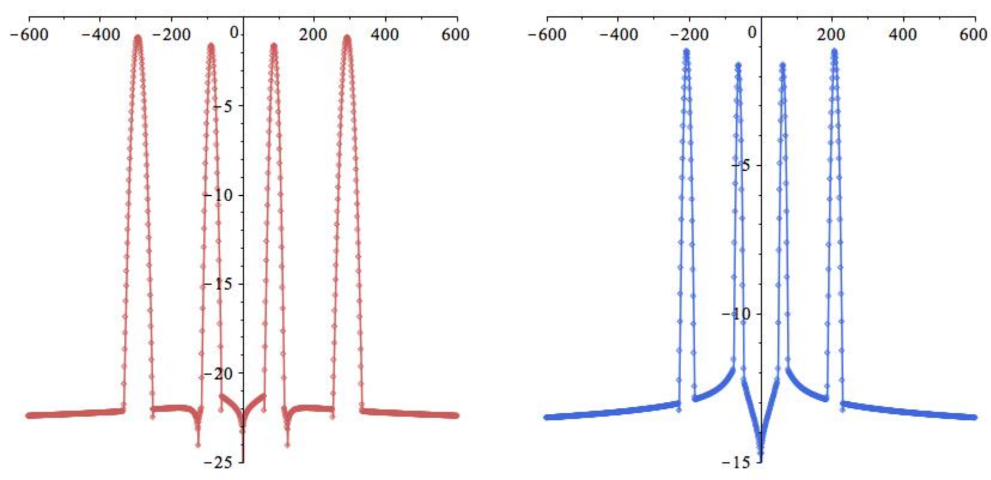

Figure 4.1: The size of stretched Fourier coefficients for (4.1) using $\lambda \approx 9.1986$ (on the left) and $\lambda \approx 6.5044$.

A more sophisticated approach is available once f is a known linear combination of wave packets, of the form (for simplicity, in one dimension)

$$f(x) = \sum_{\ell=1}^{L} \kappa_\ell \mathrm{e}^{-\alpha_\ell (x-\gamma_\ell)^2} \varphi_\ell(x),$$

where $\alpha_1, \ldots, \alpha_L > 0$. In a sufficiently large interval the decay of f is determined by the *least* α_ℓ and the latter serves as a good rule of thumb in choosing λ using (2.8) – all this provided that the γ_ℓs do not differ drastically, otherwise we might need to enlarge the window. As a simple example, consider

$$f(x) = \frac{1}{4}\mathrm{e}^{-x^2/2}\sin(30x) + \mathrm{e}^{-(x-1)^2}\cos(100x). \tag{4.1}$$

In Fig. 4.1 we have displayed $\log_{10}|f_m^\lambda|$ for $\varepsilon = 10^{-20}$ and two choices of λ: the first implied by the $\mathrm{e}^{-x^2/2}$ term and the second by the e^{-x^2} term. After initial stage (fairly long, because of rapid oscillation) both settle down to a 'floor'. For the first case we indeed recover 10^{-20} accuracy but the second choice, while converging faster, 'hits the floor' at $\approx 10^{-13}$. This is the right order of magnitude, $\mathrm{e}^{-\lambda^2/2}/(\lambda^2/2) \approx 3 \times 10^{-11}$, but well short of the desired accuracy.

Insofar as expansions in Hermite polynomials and functions are concerned, a practical algorithm based on the work of Section 3 requires a great deal of further fine tuning. Recall that connection coefficients for Hermite polynomials decay rapidly but the computation of connection coefficients for Hermite functions requires a procedure paying heed to their attenuation – a procedure which is also beneficial for Hermite polynomials. This requires taking the nature of f – its smoothness and rate of decay for $|x| \gg 1$ – into account, both to fashion sensible truncation rules in (3.2) and minimise the cost.

It is evident from Fig. 3.3 that, upon attenuation, connection coefficients behave fairly predictably. In particular, the $\check{a}_{k,m}^{\mathsf{F}}$s tend to lie asymptotically on certain simple curves. It should not be difficult to analyse further this phenomenon using asymptotic expansions of Hermite polynomials. Yet, this being marginal to the main concerns of this paper, we leave it to further research.

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A Discrete Fourier Transform and stretched Fourier expansions

One of the reasons for the extraordinary power of spectral methods is that, once the function F is periodic and analytic in an open complex strip surrounding the interval $[-1,1]$, the Discrete Fourier Transform (DFT)

$$\tilde{F}_{m,N} = \frac{1}{2N} \sum_{k=-N+1}^{N} F\left(\frac{k}{N}\right) \omega_{2N}^{-mk}, \qquad -N+1 \le m \le N, \tag{A.1}$$

where $\omega_M = \exp(2\pi\mathrm{i}/M)$ is the Mth primitive root of unity, is an extraordinarily good approximation to the Fourier coefficient $\hat{F}_m$. More precisely, there exist $c, \sigma > 0$ such that for $N \gg 1$

$$|\tilde{F}_{m,N} - \hat{F}_m| \le c\,\mathrm{e}^{-\sigma N}, \qquad -N+1 \le m \le N$$

(Henrici 1979). To complete our case for stretched Fourier expansions as a viable approximation tool on the real axis, we demonstrate in this appendix that this exponentially-small bound remains basically true once $F(x) = f(\lambda x)$, $|f(\pm\lambda)|$ is small and

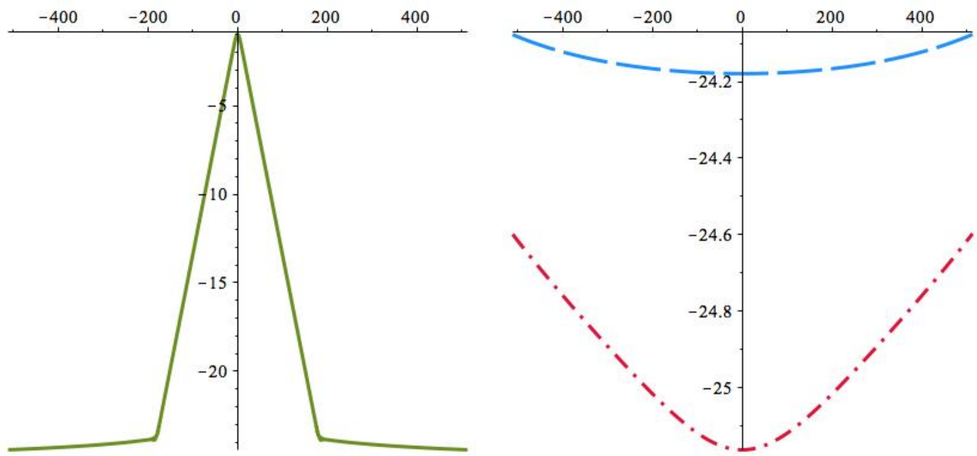

Figure A.1: Quadrature errors for $f(x) = \mathrm{e}^{-x^2/2}/\left(1+x+x^2\right)$ with $\lambda = \sqrt{2\mathrm{W}(10^{20})}$ and $N = 512$. On the left $\log_{10}|\hat{F}_m|$ and on the right $\log_{10}|\hat{F}_{m,N} - \hat{F}_m|$ for standard (dashed line) and centred (dot-dashed line) coefficients.

the choice of λ and N is such that we are within the conditions for the 'sombrero phenomenon' from Section 2.

While the standard quadrature points still produce reasonable results in practical experiments, it is favourable to replace (A.1) by *centred quadrature points,*

$$\tilde{F}_{m,N} = \frac{1}{2N} \sum_{k=-N+1}^{N} F\left(\frac{k-\frac{1}{2}}{N}\right) \omega_{2N}^{-m(k-\frac{1}{2})}, \qquad -N+1 \le m \le N. \tag{A.2}$$

On a very practical level, it consistently gives somewhat better results in our numerical tests, cf. Fig A.1. Mathematically, spectral speed of convergence is maintained, while centred points allow for an easy proof of the decay of quadrature error, which cannot be easily adapted to standard DFT (A.1). Needless to say, exactly like standard DFT, (A.3) can be computed by Fast Fourier Transform in $\mathcal{O}(N \log N)$ operations.

Let F be analytic in an open strip about $[-1,1]$. Therefore its Fourier expansion is convergent,

$$\sum_{\ell=-\infty}^{\infty} \hat{F}_\ell \, \mathrm{e}^{\pi \mathrm{i} \ell x} = F(x), \qquad x \in (-1,1).$$

Substituting into (A.3), we find the aliasing

$$\begin{aligned}\hat{F}_{m,N} &= \frac{1}{2N} \sum_{k=-N+1}^{N} \sum_{\ell=-\infty}^{\infty} \hat{F}_\ell \, \omega_{2N}^{(\ell-m)(k-\frac{1}{2})} = \frac{1}{2N} \sum_{k=-N+1}^{N} \sum_{\ell=-\infty}^{\infty} \hat{F}_{m+\ell} \, \omega_{2N}^{\ell(k-\frac{1}{2})} \\ &= \sum_{\ell=-\infty}^{\infty} \hat{F}_{m+\ell} \, \frac{\omega_{2N}^{-l/2}}{2N} \sum_{k=-N+1}^{N} \omega_{2N}^{\ell k} = \sum_{\ell=-\infty}^{\infty} (-1)^\ell \hat{F}_{m+2\ell N},\end{aligned}$$

because

$$\frac{1}{2N}\sum_{k=-N+1}^{N}\omega_{2N}^{\ell k}=\begin{cases}1, & \ell=0 \bmod 2N,\\ 0, & \text{otherwise.}\end{cases}$$

Thus the error is

$$\hat{F}_{m,N}-\hat{F}_m=\sum_{\ell\neq 0}\hat{F}_{m+2\ell N} \tag{A.3}$$

Once F is periodic, this automatically proves the decay because Fourier coefficients converge (at least) exponentially fast. Yet, in our case $F(x)=f(\lambda x)$ is not periodic, while $F(\pm 1)$ is very small.

Lemma 7 *Suppose that the function f obeys the conditions of Lemma 2. Then, with the notation of that lemma,*

$$|\hat{F}_{m,N}-\hat{F}_m|\leq\frac{\rho}{\pi}\frac{4N}{4N^2-m^2}+\frac{4\sigma}{\mathrm{e}^{\pi Nr/\lambda}-1},\qquad |m|\leq N-1. \tag{A.4}$$

Proof Our starting point is the explicit expression (A.3) of the error,

$$|\hat{F}_{m,N}-\hat{F}_m|\leq\left|\sum_{\ell=1}^{\infty}(-1)^\ell\hat{F}_{m+2\ell N}\right|+\left|\sum_{\ell=1}^{\infty}(-1)^\ell\hat{F}_{m-2\ell N}\right|$$

and we proceed by establishing uniform bounds on the finite sums with $n+1$ terms

$$\left|\sum_{\ell=1}^{n}(-1)^\ell\hat{F}_{m+2\ell N}\right| \text{ and } \left|\sum_{\ell=1}^{n}(-1)^\ell\hat{F}_{m-2\ell N}\right|.$$

From the definition of the Fourier coefficients we find

$$\begin{aligned}\sum_{\ell=1}^{n}(-1)^\ell\hat{F}_{m+2\ell N}&=\frac{1}{2\lambda}\int_{-\lambda}^{\lambda}f(z)\,\mathrm{e}^{-\mathrm{i}\pi(m+2N)z/\lambda}\sum_{\ell=0}^{n-1}\left(-\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}\right)^\ell\,\mathrm{d}z\\&=\frac{1}{2\lambda}\int_{-\lambda}^{\lambda}f(z)\,\mathrm{e}^{-\mathrm{i}\pi(m+2N)z/\lambda}\,\frac{1-\left(-\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}\right)^n}{1+\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}}\,\mathrm{d}z\end{aligned}$$

We deform the integration to the contour $\partial\mathcal{S}_r$ along its lower part $\Gamma^-=\cup_{j=1}^3\Gamma_j^-$. Thus, for any n,

$$\left|\sum_{\ell=1}^{n}(-1)^\ell\hat{F}_{m+2\ell N}\right|\leq\frac{1}{2\lambda}\int_{\Gamma^-}|f(z)|\left|\mathrm{e}^{-\mathrm{i}\pi(m+2N)z/\lambda}\right|\cdot\left|\frac{1-\left(-\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}\right)^n}{1+\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}}\right|\mathrm{d}z$$

Looking at the path integral in greater detail, we find

$$\begin{aligned}&\frac{1}{2\lambda}\int_{\Gamma_1^-}|f(z)|\left|\mathrm{e}^{-\mathrm{i}\pi(m+2N)z/\lambda}\right|\cdot\left|\frac{1-\left(-\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}\right)^n}{1+\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}}\right|\mathrm{d}z\\&\leq\frac{\rho}{2\lambda}\int_0^r\mathrm{e}^{-\pi(m+2N)y/\lambda}\left|\frac{1-\left(-\mathrm{e}^{-\pi 2Ny/\lambda}\right)^n}{1+\mathrm{e}^{-\pi 2Ny/\lambda}}\right|\mathrm{d}y\\&\leq\frac{\rho}{2\pi(2N+m)}\end{aligned}$$

– likewise, the integral along Γ_3^- yields the same bound. For the remaining part

$$\frac{1}{2\lambda}\int_{\Gamma_2^-}|f(z)|\left|\mathrm{e}^{-\mathrm{i}\pi(m+2N)z/\lambda}\right|\left|\frac{1-\left(-\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}\right)^n}{1+\mathrm{e}^{-\mathrm{i}\pi 2Nz/\lambda}}\right|\mathrm{d}z \leq 2\sigma\,\frac{\mathrm{e}^{-\pi(m+2N)r/\lambda}}{1-\mathrm{e}^{-\pi 2Nr\lambda}}.$$

Hence this shows that for $|m| \leq N$

$$\left|\sum_{\ell=1}^{\infty}(-1)^\ell \hat{F}_{m+2\ell N}\right| \leq \frac{\rho}{\pi(2N+m)}+\frac{2\sigma}{\mathrm{e}^{\pi Nr/\lambda}-1}.$$

The second sum is likewise deformed along the upper contour $\cup_{j=1}^3\Gamma_j^+$ and can be similarly bounded by

$$\left|\sum_{\ell=1}^{\infty}(-1)^\ell \hat{F}_{m-2\ell N}\right| \leq \frac{\rho}{\pi(2N-m)}+\frac{2\sigma}{\mathrm{e}^{\pi Nr/\lambda}-1}.$$

The bound (A.4) follows. □

Using the quadrature rule (A.1), we find along $\Gamma_1^\pm$ and $\Gamma_3^\pm$ the term

$$\left|\frac{1-\left(\mathrm{e}^{-\pi 2Ny/\lambda}\right)^n}{1-\mathrm{e}^{-\pi 2Ny/\lambda}}\right|$$

instead of

$$\left|\frac{1-\left(-\mathrm{e}^{-\pi 2Ny/\lambda}\right)^n}{1+\mathrm{e}^{-\pi 2Ny/\lambda}}\right|,$$

which we cannot control uniformly over n.

As we assume a rapidly decaying function along the real axis, we can under suitable extra assumptions control the error in (A.1) by the result for (A.3) up to some additional boundary terms.