The computation of the spectra of highly oscillatory Fredholm integral operators

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November 30, 2009

Abstract

We are concerned with the computation of the spectra of highly oscillatory Fredholm problems, in particular with the Fox-Li operator

$$\int_{-1}^{1} f(x) e^{i\omega(x-y)^2} dx = \lambda f(y), \qquad -1 \le y \le 1,$$

where $\omega\gg 1$. Our main tool is the finite section method: an eigenfunction is expanded in an orthonormal basis of the underlying space, resulting in an algebraic eigenvalue problem. We consider two competing bases: a basis of Legendre polynomials and a basis consisting of modified Fourier functions (cosines and shifted sines), and derive detailed asymptotic estimates of the rate of decay of the coefficients.

Although the Legendre basis enjoys in principle much faster convergence, this does not lead to much smaller matrices. Since the computation of Legendre coefficients is expensive, while modified Fourier coefficients can be computed efficiently with FFT, we deduce that modified Fourier expansions, implemented in a manner that takes advantage of their structure, present a considerably more effective tool for the computation of highly oscillatory Fredholm spectra.

1 Introduction

Our understanding of highly oscillatory phenomena and their computation has advanced in leaps and bounds in the last decade. In particular, the subject matter of highly oscillatory quadrature is, to all intents and purposes, satisfactorily understood and there exists a wealth of efficient and affordable numerical methods for integrals of the form

$$\int_{\Omega} f(\boldsymbol{x}) e^{i\omega g(\boldsymbol{x})} dx,$$

where Ω is a multivariate domain and $\omega\gg 1$ (Huybrechs & Vandewalle 2006, Iserles & Nørsett 2005, Olver 2006). This has led to a wealth of applications in rapid approximation of functions (Huybrechs, Iserles & Nørsett 2007, Huybrechs, Iserles & Nørsett 2009, Iserles & Nørsett 2008, Iserles & Nørsett 2007) and in the numerical analysis of highly oscillatory differential equations (Adcock 2008, Condon, Deaño & Iserles 2008, Iserles 2002, Khanamirian 2008). In this paper we attempt to apply similar methodology to the computation of spectra of highly oscillatory Fredholm operators, of a form ubiquitous in laser theory.

An excellent early reference to spectral problems occurring in the modelling of laser resonators is (Cochran & Hinds 1974). The underlying problem is to compute the spectrum $\sigma(\mathcal{F}_{\omega})$ of a complex-valued integral operator

$$\mathcal{F}_{\omega}[f] = \int_{-1}^{1} f(x) e^{i\omega g(x,y)} dx, \qquad \omega \gg 1,$$
(1.1)

where the *oscillator* g is a real function: important examples of oscillators, which run through this paper, are $g(x,y)=(x-y)^2$ (the Fox–Li operator) and $g(x,y)=(x-y)^4$, while the case g(x,y)=|x-y| was the subject of (Brunner, Iserles & Nørsett 2008). The spectrum in the case g(x,y)=xy was completely determined in (Cochran & Hinds 1974).

It follows readily from standard theory of Fredholm operators (cf. for example (Atkinson 1997)) that \mathcal{F}_{ω} is compact, hence $\sigma(\mathcal{F}_{\omega})$ is a point spectrum with a single accumulation point at the origin. However, being complex-symmetric, the operator is not self-adjoint and standard Hilbert–Schmidt theory is not applicable.

Bearing in mind the importance of equations (1.1) in laser engineering, the state of the theory and computation of their spectra is deeply disappointing. The pseudo-spectrum of the Fox-Li operator has been determined by Henry Landau (1977/78) and its physical features discussed at great detail by Sir Michael Berry and his co-workers in (Berry 2001, Berry 2003, Berry, Strom & van Saarlos 2001). However, both mathematical analysis and effective computational methods for the Fox-Li operator, to say nothing of more general problems (1.1), is woefully inadequate. This, we should perhaps add, is not for a lack of structure. Fig. 1.2 displays the spectra for the Fox-Li oscillator $g(x,y) = (x-y)^2$ and for $g(x,y) = (x-y)^4$ and frequency $\omega = 100$. In both cases it is clear that, consistently with theory, eigenvalues accumulate at the origin, but evidently the structure of the spectrum is considerably richer. In both cases eigenvalues appear to lie on spiral curves which approach the origin fairly rapidly – yet a formula for these spirals, even in an asymptotic form, is unknown.

Other oscillators, e.g. g(x,y) = |x - y| or g(x,y) = xy, do not produce spirals but their spectra are structured as well – cf. (Brunner et al. 2008) and (Cochran & Hinds 1974) respectively. In particular, the spectrum for g(x,y) = |x - y|, as displayed in Fig. 1.1, lies

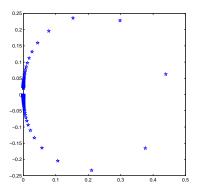


Figure 1.1: The spectrum for g(x, y) = |x - y| with $\omega = 100$.

asymptotically on the segment of the complex circle $|z-\frac{1}{2}|=\frac{1}{2}$: the eigenvalues $\{\lambda_m\}_{m=1}^\infty$ commence in the upper complex half plane, at a distance $\mathcal{O}(\omega^{-1})$ from the origin, continue within $\mathcal{O}(\omega^{-1})$ from the circle until, within the intermediate asymptotic regime, they meander away – only to return to within $\mathcal{O}(m^{-6})$ from the circle for $m\gg\omega$ and approach the origin in the lower half plane.

The general picture is complicated and fairly sensitive to the choice of the oscillator. This is demonstrated in Fig. 1.3, where the oscillator $g(x,y)=\cos[\frac{1}{2}\pi(x-y)]$ results in an 'drunken spiral', while the eigenvalues corresponding to $g(x,y)=\cos[\pi(x-y)]$ (more on these soon) lie on real and imaginary axes. For some oscillators it is difficult to discern a pattern: cf. Fig. 1.4, where we have let $g(x,y)=\sin[(x-y)^2]$. Another example is provided by $g(x,y)=\sin[\kappa(x-y)]$ for $\kappa\neq 0$: once the spectral problem for the operator \mathcal{F}_{ω} is approximated by an algebraic eigenvalue problem $A\mathbf{f}=\lambda\mathbf{f}$ (as explained in Section 2), we have $A_{n,m}=\bar{A}_{m,n}, m,n\in\mathbb{Z}_+$, the system is Hermitian and all eigenvalues are real. By this stage it is too early to venture even a conjecture on more general patterns of behaviour of the spectra of (1.1).

Although this is tangential to the narrative of this paper, it is interesting (and fairly easy) to explain the cross-like structure in Fig. 1.3 and, indeed, identify the spectrum for the oscillator $g(x) = \cos[\pi(x-y)]$: our claim is that the eigenvalues are $\lambda_n = 2\mathrm{i}^n\mathrm{J}_n(\omega)$ with the corresponding eigenfunctions $f_n(x) = \mathrm{e}^{\mathrm{i} n x}$, $n \in \mathbb{Z}$. Here J_n is the nth Bessel function. To prove this assertion we use identities 9.1.44–45 in (Abramowitz & Stegun 1964, p.361) to argue that

$$e^{i\omega\cos[\pi(x-y)]} = J_0(\omega) + 2\sum_{m=1}^{\infty} i^m J_m(\omega)\cos[\pi m(x-y)].$$

Therefore for every $n \in \mathbb{Z}$

$$\mathcal{F}_{\omega}[e^{i\pi ny}] = \int_{-1}^{1} e^{i\pi nx} \left\{ J_0(\omega) + \sum_{m=1}^{\infty} i^m J_m(\omega) [e^{i\pi m(x-y)} + e^{-i\pi m(x-y)}] \right\} dx$$

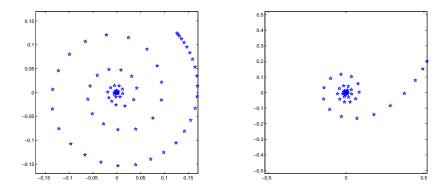


Figure 1.2: The spectra for $g(x,y)=(x-y)^2$ and $g(x,y)=(x-y)^4$ with $\omega=100$.

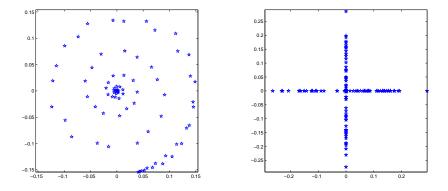


Figure 1.3: The spectra for $g(x,y)=\cos[\frac{1}{2}\pi(x-y)]$ and $g(x,y)=\cos[\pi(x-y)]$ with $\omega=100$.

$$= \int_{-1}^{1} e^{i\pi nx} dx J_0(\omega) + \sum_{m=1}^{\infty} i^m J_m(\omega) e^{-i\pi my} \int_{-1}^{1} e^{i\pi(n+m)x} dx$$
$$+ \sum_{m=1}^{\infty} i^m J_m(\omega) e^{i\pi my} \int_{-1}^{1} e^{i\pi(n-m)x} dx = 2i^n J_n(\omega) e^{i\pi ny}.$$

Note that $\lambda_{2n} \in \mathbb{R}$, $\lambda_{2n+1} \in \mathbb{R}$ and that $\lambda_{|n|}$ tends to zero as $n \to \infty$ spectrally fast.

This paper is devoted to efficient computational algorithms for the calculation of the eigenvalues of the operator (1.1) in the generic case, when the latter cannot be derived in a closed form. It is usual in the computation of spectra of integral operators to employ the *finite section method* (Arveson 1994, Hagen, Roch & Silbermann 2001). Thus, let $\Phi = \{\phi_m\}_{m \in \mathbb{Z}_+}$ be an

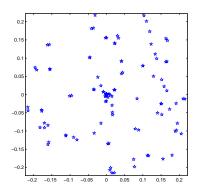


Figure 1.4: The spectrum for $g(x, y) = \sin[(x - y)^2]$ with $\omega = 100$.

orthonormal basis of $L_2[-1,1]$. Expanding an eigenfunction f in this basis,

$$f(x) = \sum_{m=0}^{\infty} f_m \phi_m(x),$$

substitution into (1.1) and integration in $y \in [-1, 1]$ result in the infinite-dimensional algebraic eigenvalue problem

$$\sum_{m=0}^{\infty} A_{n,m} f_m = \lambda f_n, \qquad n \in \mathbb{Z}_+,$$

where

$$A_{n,m} = \int_{-1}^{1} \int_{-1}^{1} \phi_n(x)\phi_m(y)e^{i\omega g(x,y)} dx dy, \qquad m, n \in \mathbb{Z}_+.$$
 (1.2)

The standard procedure, justified by the compactness of the underlying problem, is to truncate the matrix A and solve the resulting finite-dimensional algebraic eigenvalue problem by the very efficient methods of numerical linear algebra. The challenge is to choose a basis Φ satisfying two desiderata: rapid convergence of the truncated expansion to an eigenfunction (since this means that the underlying finite matrix need not be excessively large) and affordable computation of the double integrals (1.2). An aggravating factor is the presence of two different mechanisms that generate high oscillation in (1.2). Firstly, we are interested in large values of ω ; secondly for large m (smooth) orthogonal functions ϕ_m are themselves highly oscillatory. This competition between two forms of high oscillation is an important organising principle underlying our work.

An obvious alternative to the finite section method is to discretize the integral in (1.1) by quadrature. Thus, given 2N+1 quadrature points

$$-1 \le c_{-N} < c_{-N+1} < \dots < c_N \le 1$$

and corresponding weights $b_{-N}, b_{-N+1}, \dots, b_N$, we can approximate the spectral problem for (1.1) by the finite-dimensional algebraic eigenvalue problem

$$\sum_{m=-N}^{N} f_m e^{i\omega g(c_m, c_n)} = \lambda f_n, \qquad n = -N, -N+1, \dots, N,$$
(1.3)

where $f_m \approx f(c_m)$. (In principle, we can bring (1.3) into the formalism of the finite section approach, letting the orthogonal functions ϕ_m be delta functions, but this helps little in understanding this method.) Clearly, (1.3) belabours under three disadvantages. Firstly, the (m,n) element of the matrix whose eigenvalues we seek is $\mathcal{O}(N^{-1})$, hence we need to choose very large values of N to attain good accuracy. Secondly, once ω is large, we need to take truly huge value of N, so that integration occurs in a non-oscillatory regime. (The current approach denies us the benefits of highly oscillatory quadrature.) Finally, once N is very large, although it is possible to compute rapidly nodes and weights associated with nontrivial quadrature schemes (Glaser, Liu & Rokhlin 2007), efficient implementation of, say, Gaussian rules is impractical. Therefore, we are compelled in practice to choose equally-spaced nodes $c_m = m/N$, with weights $b_m \equiv 1/(N+\frac{1}{2})$, thus denied the benefits of such quadrature methods as Gauss-Legendre or Clenshaw-Curtis.

The plan of this paper is as follows. In Section 2 we address the most natural approach to the choice of the basis Φ , namely Legendre polynomials. Although general considerations originating in the theory of spectral methods indicate very rapid convergence as the size of a section increases, it turns out that this approach has a number of substantive disadvantages. This motivates our exploration in Section 3 of the alternative of using expansions in exponentials, focusing on modified Fourier expansion. Finally, in Section 4 we show how the idea of hyperbolic cross leads to substantial cost savings once we use modified Fourier expansions.

2 Expansion in Legendre polynomials

2.1 An explicit formula

Choosing the Legendre basis $\phi_m(x) = (m + \frac{1}{2})^{\frac{1}{2}} P_m(x), m \in \mathbb{Z}_+$, we have

$$A_{m,n} = (m + \frac{1}{2})^{\frac{1}{2}} (n + \frac{1}{2})^{\frac{1}{2}} \int_{-1}^{1} \int_{-1}^{1} P_m(x) P_n(y) e^{i\omega g(x,y)} dx dy$$

$$= (m + \frac{1}{2})^{\frac{1}{2}} (n + \frac{1}{2})^{\frac{1}{2}} \int_{-1}^{1} \int_{-1}^{1} P_m(x) P_n(y) K_{\omega}(x,y) dx dy$$
(2.1)

for all $m,n\in\mathbb{Z}_+$, where $K_\omega(x,y)=\mathrm{e}^{\mathrm{i}\omega g(x,y)}$. It follows from standard theory of spectral methods (cf. (Hesthaven, Gottlieb & Gottlieb 2007) or any number of similar references) that, provided $g\in\mathrm{C}^\infty([-1,1]^2)$, the coefficients $A_{m,n}$ decay at a spectral speed as $m+n\to\infty$, that is faster than a reciprocal of any polynomial in m and n.

We let

$$A_{m,n} = (m + \frac{1}{2})^{\frac{1}{2}} (n + \frac{1}{2})^{\frac{1}{2}} \tilde{A}_{m,n}$$

and work in the future with the somewhat simpler coefficients $\tilde{A}_{m,n}$.

It is convenient by this stage to generalize a univariate formula for Legendre expansions to our setting. Given function

$$f(z) = \sum_{n=0}^{\infty} \frac{f_n}{n!} z^n,$$

analytic in [-1, 1], it is true that

$$f(x) = \sum_{n=0}^{\infty} (2n+1) \sum_{k=0}^{\infty} \frac{f_{n+2k}}{2^{n+2k} k! (\frac{3}{2})_{n+k}} P_n(x)$$
 (2.2)

(Rainville 1960, p.181). Here $(z)_n$ is the *Pochhammer symbol*: $(z)_0 = z$ and $(z)_n = z(z+n-1)$ for $n \in \mathbb{N}$. Since $\int_{-1}^{1} P_n^2(x) dx = n + \frac{1}{2}$, it thus follows that

$$\int_{-1}^{1} f(x) P_n(x) dx = \sum_{k=0}^{\infty} \frac{f_{n+2k}}{2^{n+2k-1} k! (\frac{3}{2})_{n+k}}, \qquad n \in \mathbb{Z}_+.$$
 (2.3)

Likewise, suppose that the kernel K_{ω} is an analytic function of $(x,y) \in [-1,1]^2$,

$$K_{\omega}(x,y) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{r_{k,l}}{k!l!} x^k y^l, \qquad x, y \in [-1, 1],$$

where $r_{k,l} = \partial_x^k \partial_y^l K_\omega(0,0)$. Generalizing (2.3) to this setting is straightforward,

$$\tilde{A}_{m,n} = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{r_{m+2k,n+2l}}{2^{m+n+2(k+l-1)}k!l!(\frac{3}{2})_{m+k}(\frac{3}{2})_{n+l}}, \qquad m, n \in \mathbb{Z}_{+}.$$
 (2.4)

An important special case is that of an *Abel kernel* $K_{\omega}(x,y) = \rho_{\omega}(x-y)$, e.g. the Fox–Li operator. In that case, letting $\rho_k = \rho^{(k)}(0)$, we have

$$K_{\omega}(x,y) = \sum_{l=0}^{\infty} \frac{\rho_l}{l!} (x-y)^l = \sum_{l=0}^{\infty} \frac{\rho_l}{l!} \sum_{k=0}^{l} \binom{l}{k} (-1)^{l-k} x^k y^{l-k}$$
$$= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^l \rho_{k+l}}{k! l!} x^k y^l.$$

Therefore $r_{k,l} = (-1)^l \rho_{k+l}$ and (2.4) simplifies to

$$\tilde{A}_{m,n} = (-1)^n \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{\rho_{m+n+2(k+l)}}{2^{m+n+2(k+l-1)}k! l! (\frac{3}{2})_{m+k} (\frac{3}{2})_{n+l}}, \qquad m, n \in \mathbb{Z}_+.$$
 (2.5)

The explicit formulæ (2.4) and (2.5) are of limited use. Even if derivatives at the origin are freely and easily available, explicit summation is expensive and likely to be ill conditioned because – as we soon see – it involves terms of radically different magnitude. The situation is considerably worse if derivatives are computed numerically, not just because of the very considerable additional expense but also since computation of derivatives is itself a notoriously ill conditioned procedure.

The sobering truth is that no computational procedure is truly effective in the computation of Legendre coefficients $A_{m,n}$. Perhaps the most effective is to discretize the integral at Chebyshev points and use fast algorithms to compute the underlying quadrature: this is essentially a combination of Clenshaw–Curtis quadrature with FFT (Clenshaw & Curtis 1960, Potts, Steidl & Tasche 1998), but its origins can be traced to the work of Fejér (Fejér 1933a, Fejér 1933b). Yet, even using such rapid algorithms we would require in a bivariate setting an excessively large volume of computations. This is precisely the reason why Legendre expansions are typically avoided in spectral methods, although arguably the uniform Legendre measure is the natural one in defining the underlying inner product. Instead, it is usual to employ either Chebyshev expansions (which can be computed very effectively with FFT) or Legendre collocation. In the current setting, though, we cannot impose by fiat the Chebyshev measure are compelled (at least in this setting) to expand in Legendre polynomials.

In special cases we can further massage explicit formulæ (2.4) or (2.5) to render them suitable for computation. An important example is provided by the Fox–Li operator.

2.2 The Fox-Li operator

Letting $\rho(x) = e^{i\omega x^2}$, $x \in [-2, 2]$, we have

$$\rho_{2m} = \frac{(2m)!}{m!} (i\omega)^m, \quad \rho_{2m+1} = 0, \qquad m \in \mathbb{Z}_+.$$

Therefore, substituting in (2.5),

$$\begin{split} \tilde{A}_{2m,2n} &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(2m+2n+2k+2l)! (\mathrm{i}\omega)^{m+n+k+l}}{4^{m+n+k+l-1}k! l! (m+n+k+l)! (\frac{3}{2})_{2m+k} (\frac{3}{2})_{2m+l}} \\ &= \sum_{k=0}^{\infty} \sum_{r=k}^{\infty} \frac{(2m+2n+2r)! (\mathrm{i}\omega)^{m+n+r}}{4^{m+n+r-1}k! (r-k)! (m+n+r)! (\frac{3}{2})_{2m+k} (\frac{3}{2})_{2n+r-k}} \\ &= \sum_{r=0}^{\infty} \frac{(2m+2n+2r)!}{4^{m+n+r-1}(m+n+r)! r!} \left[\sum_{k=0}^{r} \binom{r}{k} \frac{1}{(\frac{3}{2})_{2m+k} (\frac{3}{2})_{2n+r-k}} \right] (\mathrm{i}\omega)^{m+n+r} \\ &= \sum_{r=0}^{\infty} \frac{(2m+2n+2r)!}{4^{m+n+r-1}(m+n+r)! r!} v_r^{m,n} (\mathrm{i}\omega)^{m+n+r}. \end{split}$$

Since

$$\binom{r}{k} = (-1)^k \frac{(-r)_k}{k!}, \qquad (\frac{3}{2})_{2m-k} = (\frac{3}{2})_{2m} (\frac{3}{2} + 2m)_k,$$
$$(\frac{3}{2})_{2n+r-k} = \frac{(-1)^k (\frac{3}{2})_{2n+r}}{(-\frac{1}{2} - 2n - r)_k},$$

we have

$$v_r^{m,n} = \frac{1}{(\frac{3}{2})_{2m}(\frac{3}{2})_{2n+r}} {}_{2}F_{1} \left[\frac{-r, -\frac{1}{2} - 2n - r}{\frac{3}{2} + 2m}; 1 \right]$$

$$= \frac{1}{(\frac{3}{2})_{2m}(\frac{3}{2})_{2n+r}} \frac{\Gamma(\frac{3}{2}+2m)(2m+2n+2r+1)!}{\Gamma(\frac{3}{2}+2m+r)(2m+2n+r+1)!}$$
$$= \frac{1}{(\frac{3}{2})_{2m+r}(\frac{3}{2})_{2n+r}} \frac{(2m+2n+2r+1)!}{(2m+2n+r+1)!},$$

where ${}_p\mathrm{F}_q$ denotes a (p,q) generalized hypergeometric function (Rainville 1960, p.73). We deduce that

$$\tilde{A}_{2m,2n} = \sum_{r=0}^{\infty} \frac{(2m+2n+2r)!(2m+2n+2r+1)!(\mathrm{i}\omega)^{m+n+r}}{4^{m+n+r-1}(m+n+r)!r!(2m+2n+r+1)!(\frac{3}{2})_{2m+r}(\frac{3}{2})_{2n+r}}.$$

But

$$\frac{(2m+2n+2r)!}{4^{m+n+r-1}(m+n+r)!} = 4(\frac{1}{2})_{m+n+r},$$
$$\frac{(2m+2n+2r+1)!}{(2m+2n+r+1)!} = \frac{4^r(m+n+1)_r(m+n+\frac{3}{2})_r}{(2m+2n+2)_r}$$

consequently, after some elementary algebra,

$$\tilde{A}_{2m,2n} = \frac{4(\mathrm{i}\omega)^{m+n}(\frac{1}{2})_{m+n}}{(\frac{3}{2})_{2m}(\frac{3}{2})_{2n}} {}_{3}\mathrm{F}_{3} \left[\begin{array}{c} m+n+\frac{1}{2}, m+n+1, m+n+\frac{3}{2}; \\ 2m+2n+2, 2m+\frac{3}{2}, 2n+\frac{3}{2}; \end{array} \right] 4\mathrm{i}\omega \right].$$

Likewise,

$$\tilde{A}_{2m+1,2n+1} = -\frac{4(\mathrm{i}\omega)^{m+n+1}(\frac{1}{2})_{m+n+1}}{(\frac{3}{2})_{2m+1}(\frac{3}{2})_{2n+1}} {}_{3}F_{3} \left[\begin{array}{c} m+n+\frac{3}{2}, m+n+2, m+n+\frac{5}{2}; \\ 2m+2n+4, 2m+\frac{5}{2}, 2n+\frac{5}{2}; \end{array} \right] \mathrm{d}\omega \right].$$

Therefore, for every $m, n \in \mathbb{Z}_+$, m + n even,

$$\tilde{A}_{m,n} = \frac{4(-1)^n (\mathrm{i}\omega)^{\frac{1}{2}(m+n)} (\frac{1}{2})_{\frac{1}{2}(m+n)}}{(\frac{3}{2})_m (\frac{3}{2})_n} {}_3F_3 \begin{bmatrix} \frac{m+n}{2} + \frac{1}{2}, \frac{m+n}{2} + 1, \frac{m+n}{2} + \frac{3}{2}; \\ m+n+2, m+\frac{3}{2}, n+\frac{3}{2}; \end{bmatrix} (2.6)$$

Since, trivially, $\tilde{A}_{m,n}=0$ for all $m,n\in\mathbb{Z}_+$, m+n odd, we have all the coefficients of the matrix A in an explicit form – except that the calculation of generalized hypergeometric functions is neither trivial nor fast even with modern software.

2.3 Asymptotics of Fox-Li coefficients

It is central to the subject matter of this paper that coefficients $A_{m,n}$ possess two kinds of asymptotics which are germane to the understanding of the finite section method: $\omega \to \infty$ for fixed m,n (large- ω asymptotics) and $m+n\to\infty$ for fixed ω (large-(m,n) asymptotics). In this subsection we address the issue of large-(m,n) asymptotics for Legendre coefficients. Our starting point is the explicit representation (2.6).

Theorem 1 For every $n \in \mathbb{Z}_+$ it is true that

$$\tilde{A}_{n,n} = \frac{(-1)^n i^n \pi^{\frac{1}{2}}}{\omega^{\frac{1}{2}}} \int_0^2 \frac{e^{i\omega x}}{x} J_{n+\frac{1}{2}}(\omega x) dx, \tag{2.7}$$

$$\tilde{A}_{n-s,n+s} = \frac{(-1)^{n+1} i^n \pi^{\frac{1}{2}}}{2\omega^{\frac{1}{2}}} \int_0^2 \theta_s(x) e^{i\omega x} J_{n+\frac{1}{2}}(\omega x) dx, \qquad 0 \le s \le n,$$
 (2.8)

where

$$\theta_s(x) = s_2 F_1 \begin{bmatrix} -s+1, s-1; & x \\ 2; & 2 \end{bmatrix}.$$

Proof We commence from (2.7). Letting m = n in (2.6) and using the second Kummer formula for confluent hypergeometric functions (Rainville 1960, p. 126), we have

$$\begin{split} \tilde{A}_{n,n} &= \frac{4(-1)^n (\mathrm{i}\omega)^n (\frac{1}{2})_n}{[(\frac{3}{2})_n]^2} {}_2F_2 \left[\frac{n + \frac{1}{2}, n + 1;}{2n + 2, n + \frac{3}{2};} 4\mathrm{i}\omega \right] \\ &= \frac{2(-1)^n (\mathrm{i}\omega)^n}{(\frac{3}{2})_n} \sum_{r=0}^{\infty} \frac{(n+1)_r}{r! (2n+2)_r} \frac{(4\mathrm{i}\omega)^r}{n + r + \frac{1}{2}} \\ &= \frac{(-1)^n}{4^n (\frac{3}{2})_n (\mathrm{i}\omega)^{\frac{1}{2}}} \int_0^{4\mathrm{i}\omega} \sum_{r=0}^{\infty} \frac{(n+1)_r}{r! (2n+2)_r} x^{n+r-\frac{1}{2}} \, \mathrm{d}x \\ &= \frac{(-1)^n}{4^n (\frac{3}{2})_n (\mathrm{i}\omega)^{\frac{1}{2}}} \int_0^{4\mathrm{i}\omega} x^{n-\frac{1}{2}} {}_1F_1 \left[\frac{n+1;}{2n+2;} x \right] \, \mathrm{d}x \\ &= \frac{(-1)^n 2^{\frac{1}{2}} (\frac{1}{2}\mathrm{i}\omega)^n}{(\frac{3}{2})_n} \int_0^2 x^{n-\frac{1}{2}} {}_1F_1 \left[\frac{n+1;}{2n+2;} 2\mathrm{i}\omega x \right] \, \mathrm{d}x \\ &= \frac{(-1)^n 2^{\frac{1}{2}} (\frac{1}{2}\mathrm{i}\omega)^n}{(\frac{3}{2})_n} \int_0^2 x^{n-\frac{1}{2}} {}_1F_1 \left[\frac{n+1;}{2n+2;} 2\mathrm{i}\omega x \right] \, \mathrm{d}x \\ &= \frac{(-1)^n 2^{\frac{1}{2}} (\frac{1}{2}\mathrm{i}\omega)^n}{(\frac{3}{2})_n} \int_0^2 x^{n-\frac{1}{2}} {}_1\mathrm{e}^{\mathrm{i}\omega x} {}_0\mathrm{F}_1 \left[\frac{-\mathrm{i}}{n+\frac{3}{2};} - \frac{\omega^2 x^2}{4} \right] \, \mathrm{d}x. \end{split}$$

Since

$$_{0}\mathrm{F}_{1}\left[\begin{array}{c} - ; \\ \nu + 1 ; \end{array} - \frac{x^{2}}{4} \right] = \frac{\Gamma(\nu + 1)}{(x/2)^{\nu}}\mathrm{J}_{\nu}(x)$$

(Rainville 1960, p. 108), we confirm (2.7).

Next, we choose $s \in \mathbb{N}$, whence for every $n \geq s$ (2.6) yields

$$\tilde{A}_{n-s,n+s} = \frac{4(-1)^{n+s}(i\omega)^n(\frac{1}{2})_n}{(\frac{3}{2})_{n-s}(\frac{3}{2})_{n+s}} {}_{3}F_{3} \left[\frac{n+\frac{1}{2},n+1,n+\frac{3}{2};}{2n+2,n-s+\frac{3}{2},n+s+\frac{3}{2};} 4i\omega \right]$$

$$= \frac{(-1)^{n+s}(i\omega)^n(\frac{1}{2})_n}{(\frac{1}{2})_{n-s+1}(\frac{1}{2})_{n+s+1}} \sum_{k=0}^{\infty} \frac{(n+1)_k}{k!(2n+2)_k} \frac{(n+\frac{1}{2})_k(n+\frac{3}{2})_k}{(n-s+\frac{3}{2})_k(n+s+\frac{1}{2})_k} (4i\omega)^k$$

$$= \frac{(-1)^{n+s}(i\omega)^n}{(\frac{1}{2})_{n+1}} \sum_{k=0}^{\infty} \frac{(n+1)_k}{k!(2n+2)_k} \kappa_s(n,k) (4i\omega)^k,$$

where

$$\kappa_s(n,k) = \frac{(\frac{1}{2})_n(\frac{1}{2})_{n+1}}{(\frac{1}{2})_{n-s+1}(\frac{1}{2})_{n+s+1}} \frac{(n+\frac{1}{2})_k(n+\frac{3}{2})_k}{(n-s+\frac{1}{2})_k(n+s+\frac{3}{2})_k} = \frac{(n+k+\frac{3}{2}-s)_{s-1}}{(n+k+\frac{3}{2})_s}.$$

Our claim is that $\kappa_s(n,k) = \varphi_s(n+k)$, where

$$\varphi_s(x) = \sum_{k=0}^{s-1} (-1)^{s-1-k} \frac{\alpha_{s,k}}{x+k+\frac{3}{2}}, \qquad \alpha_{s,k} = \frac{(s+k)!}{k!(k+1)!(s-k-1)!}.$$

This follows at once by representing the rational function φ_s in the form

$$\varphi_s(x) = \frac{(x + \frac{3}{2} - s)_{s-1}}{(x + \frac{3}{2})_s} = \sum_{k=0}^{s-1} (-1)^{s-1-k} \frac{\alpha_{s,k}}{x + k + \frac{3}{2}},$$

where the $\alpha_{s,k}$ s are the residues at $x=-k-\frac{3}{2}$.

We conclude that

$$\begin{split} \tilde{A}_{n-s,n+s} &= \frac{(1-)^{n+s}(\mathrm{i}\omega)^n}{(\frac{1}{2})_{n+1}} \sum_{k=0}^{\infty} \frac{(n+1)_k}{k!(2n+2)_k} \varphi_s(n+k) (4\mathrm{i}\omega)^k \\ &= \frac{(-1)^{n+1}(\mathrm{i}\omega)^n}{(\frac{1}{2})_{n+1}} \sum_{l=0}^{s-1} \frac{\alpha_{s,l}}{(4\mathrm{i}\omega)^{n+l+\frac{3}{2}}} \sum_{k=0}^{\infty} \frac{(n+1)_k}{k!(2n+2)_k} \frac{(4\mathrm{i}\omega)^{n+k+l+\frac{3}{2}}}{n+k+l+\frac{3}{2}} \\ &= \frac{(-1)^{n+1}(\mathrm{i}\omega)^n}{(\frac{1}{2})_{n+1}} \sum_{l=0}^{s-1} \frac{\alpha_{s,l}}{(4\mathrm{i}\omega)^{n+l+\frac{3}{2}}} \int_0^{4\mathrm{i}\omega} x^{n+l+\frac{1}{2}} {}_1\mathrm{F}_1 \left[\frac{n+1}{2n+2}; x \right] \mathrm{d}x \\ &= \frac{(-1)^{n+1}(\mathrm{i}\omega)^n}{(\frac{1}{2})_{n+1}} \sum_{l=0}^{s-1} \frac{\alpha_{s,l}}{2^{n+l+\frac{3}{2}}} \int_0^2 x^{n+l+\frac{1}{2}} \mathrm{e}^{\mathrm{i}\omega x} {}_0\mathrm{F}_1 \left[\frac{-;}{n+\frac{3}{2}}; -\frac{\omega^2 x^2}{4} \right] \mathrm{d}x, \end{split}$$

where we have used the second Kummer formula to convert the ${}_{1}F_{1}$ function to ${}_{0}F_{1}$. Thus, we deduce (2.8) from

$$_{0}F_{1}\left[\begin{array}{c} -;\\ n+\frac{3}{2}; \end{array} - \frac{\omega^{2}x^{2}}{4}\right] = \frac{\pi^{\frac{1}{2}}(\frac{1}{2})_{n}2^{n+\frac{1}{2}}}{\omega^{n+\frac{1}{2}}x^{n+\frac{1}{2}}} J_{n+\frac{1}{2}}(\omega x)$$

and the explicit form of $\alpha_{s,l}$.

Note that θ_s can be written as a Jacobi polynomial (Rainville 1960, p. 254),

$$\theta_s(x) = P_{s-1}^{(1,0)}(1-x),$$

although this plays no further role in our analysis.

The integral expressions (2.7) and (2.8) need to be further massaged to reveal their asymptotic behaviour for $n \to \infty$. To this end we need the following simple result.

Proposition 2 Let

$$I_n[f] = \frac{1}{2^{n+\frac{3}{2}}} \int_0^2 x^{n+\frac{1}{2}} f(x) dx, \qquad n \in \mathbb{Z}_+,$$

where $f \in C^{\infty}[0,2]$. Then

$$I_n[f] \sim \frac{f(2)}{n+\frac{1}{2}} - \frac{2f'(2)+f(2)}{(n+\frac{1}{2})^2} + \frac{4f''(2)+6f'(2)+f(2)}{(n+\frac{1}{2})^3} + \mathcal{O}(n^{-4}), \qquad n \gg 1.$$
 (2.9)

Proof Similarly to (Iserles & Nørsett 2005), we integrate by parts,

$$I_n[f] = \frac{1}{2^{n+\frac{3}{2}}} \int_0^2 f(x) e^{(n+\frac{1}{2})\log x} dx = \frac{1}{2^{n+\frac{3}{2}}} \frac{1}{n+\frac{1}{2}} \int_0^2 x f(x) \frac{d}{dx} e^{(n+\frac{1}{2})\log x} dx$$
$$= \frac{f(2)}{n+\frac{1}{2}} - \frac{1}{2^{n+\frac{3}{2}}} \frac{1}{n+\frac{1}{2}} \int_0^2 [x f'(x) + f(x)] e^{(n+\frac{1}{2})\log x} dx.$$

Two further integrations by part yield (2.9).

Theorem 3 For any fixed ω and $s \in \mathbb{N}$ and for $n \to \infty$ it is true that

$$\begin{split} \tilde{A}_{n,n} &\sim \frac{(-\mathrm{i}\omega)^n \mathrm{e}^{n+\frac{1}{2}} \mathrm{e}^{2\mathrm{i}\omega}}{2^{\frac{1}{2}} (n+\frac{1}{2})^{n+\frac{1}{2}}} \left[\frac{1}{n-\frac{1}{2}} - \frac{1+2\mathrm{i}\omega}{(n-\frac{1}{2})^2} + \frac{1+6\mathrm{i}\omega-4\omega^2}{(n-\frac{1}{2})^3} + \mathcal{O}\!\left(n^{-4}\right) \right] \\ \tilde{A}_{n-s,n+s} &\sim -\frac{(-\mathrm{i}\omega)^n \mathrm{e}^{n+\frac{1}{2}} \mathrm{e}^{2\mathrm{i}\omega}}{2^{\frac{1}{2}} (n+\frac{1}{2})^2} \left[1 - \frac{s^2 + \mathrm{i}\omega}{n+\frac{1}{2}} + \frac{\frac{1}{2}s^2(s^2+1) + 2\mathrm{i}\omega(2s^2+1) - 4\omega^2}{(n+\frac{1}{2})^2} + \mathcal{O}\!\left(n^{-3}\right) \right]. \end{split}$$

Proof Follows by easy algebra from Theorem 1, the asymptotic estimate

$$J_{\nu}(x) \sim \frac{1}{(2\pi\nu)^{\frac{1}{2}}} \left(\frac{ex}{2\nu}\right)^{\nu}$$

(Abramowitz & Stegun 1964, p.365) and the asymptotic expansion (2.9).

Theorem 3 quantifies something that we already know: as n grows, the size of the coefficients decays at spectral speed. However, it highlights a fact which is crucial to the understanding of the finite-section method for highly oscillatory Fredholm operators: the behaviour of the coefficients is determined by the competition between large-(m+n) and large- ω asymptotics. This is illustrated in Fig. 2.1, where we have plotted $-\log_{10}|\tilde{A}_{m,n}|$ for $\omega=100$, growing n and the cases m=n, m=n-2 and m=0 (in the latter case only even values of n have been displayed, since $\tilde{A}_{0,2n+1}\equiv 0$). Evidently, the size of $|\tilde{A}_{m,n}|$ drops quite sedately for a long while and then, having reached a threshold when large-(m,n) asymptotics take over, suddenly $|\tilde{A}_{m,n}|$ drops literally like a stone. For example, $|\tilde{A}_{200,200}|=6.30_{-05}$, while $|\tilde{A}_{250,250}|=1.25_{-15}$. This process is faster when descending along diagonals and somewhat slower along rows and columns of A: thus, $|\tilde{A}_{0,275}|=2.47_{-06}$ and $|\tilde{A}_{0,325}|=8.59_{-15}$.

This phenomenon is consistent for different values of ω and also for other oscillators, not just Fox–Li. Its operative implication is as follows. For the finite section method to compute eigenvalues of the infinite-dimensional operator well, we must truncate the infinite matrix A by discarding sufficiently small entries. The entries become small (very rapidly!) only once large-(m,n) asymptotics take over, and this imposes a fairly large lower bound on the size of truncated matrix A: for Fox–Li, the one instance where the large-(m,n) asymptotics are known, computational experience indicates that a good choice of dimension of A is $\approx 2\sqrt{2}\omega$. (This actually is slightly better, because for Fox–Li – and for other symmetric oscillators $g(x,y)=g(y,x)-\tilde{A}_{m,n}=0$ when m and n are of opposite parity and the matrix A can be partitioned into two matrices of half the size.)

The lesson from our analysis of Legendre expansions applied to the Fox–Li operator is twofold. Firstly, the frequency ω imposes a lower bound on the size of A which is immune

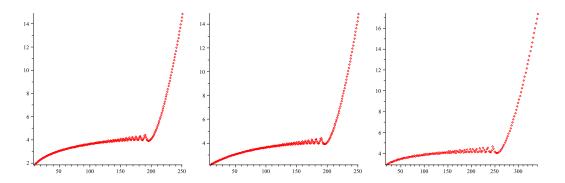


Figure 2.1: $-\log_{10}|\tilde{A}_{2m,2n}|$ for $n=0,1,\dots,250$ and (a) m=n; (b) m=n-2; (c) m=0,n even. In all cases $\omega=100$.

to the spectral decay in the size of the coefficients. Secondly, even if the $\tilde{A}_{m,n}$ s are available explicitly, their computation is time-consuming. Of course, in the general case the coefficients are not available in an explicit form and their approximate calculation is a formidable challenge to which there are currently no easy answers.

2.4 Other oscillators

It is interesting to examine Legendre coefficients $\tilde{A}_{m,n}$ in special cases when they can be computed explicitly, since this provides us with useful data toward the understanding of the general problem. This is the case even if the spectrum is explicitly known, as it is in the two following examples.

We commence by considering

$$\mathcal{F}[f] = \int_{-1}^{1} f(x) \cos \omega(x - y) \, \mathrm{d}x. \tag{2.10}$$

This does not fit into the pattern (1.1): we have real kernel of Abel type $K_{\omega}(x,y) = \cos \omega(x-y)$. Yet, the logic underlying the finite section method is still valid, as is formula (2.4). The spectrum of (2.10) can be easily evaluated since the kernel is of rank 2 and just two eigenvalues can differ from zero: they are

$$\begin{split} \lambda_1 &= 1 - \frac{\sin 2\omega}{2\omega}, \quad \text{with the eigenfunction} \quad f_1(y) = \sin \omega y, \\ \lambda_2 &= 1 + \frac{\sin 2\omega}{2\omega}, \quad \text{with the eigenfunction} \quad f_1(y) = \cos \omega y, \end{split}$$

while the invariant subspace of eigenfunctions corresponding to the infinite-multiplicity zero eigenvalue is spanned by $\sin \alpha_n y$ and $\cos \beta_n y$, $n \in \mathbb{Z}_+$, where $\alpha_n, \beta_n \neq \omega$ are solutions of the transcendental equations

$$\alpha \cot \alpha = \omega \cot \omega$$
, $\beta \tan \beta = \omega \tan \omega$.

Symmetry implies that $\tilde{A}_{m,n} = 0$ for odd m + n, while

$$\begin{split} \tilde{A}_{2m,2n} &= \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{m+n+k+l} \omega^{2(m+n+k+l)}}{4^{m+n+k+l-1} k! l! (\frac{3}{2})_{2m+k} (\frac{3}{2})_{2n+l}} \\ &= \sum_{k=0}^{\infty} \sum_{r=k}^{\infty} \frac{(-1)^{m+n+r} \omega^{2(m+n+r)}}{4^{m+n+r-1} k! (r-k)! (\frac{3}{2})_{2m+k} (\frac{3}{2})_{2n+r-k}} \\ &= \sum_{r=0}^{\infty} \frac{(-\omega^2)^{m+n+r}}{4^{m+n+r-1} r!} \sum_{k=0}^{r} \frac{r!}{k! (r-k)! (\frac{3}{2})_{2m+k} (\frac{3}{2})_{2n+r-k}}. \end{split}$$

Since

$$\frac{1}{(\frac{3}{2})_{2m+k}} = \frac{1}{(\frac{3}{2})_{2m}(2m+\frac{3}{2})_k}, \qquad \frac{r!}{(r-k)!} = (-1)^k (-r)_k,$$
$$\frac{1}{(\frac{3}{2})_{2n+r-k}} = \frac{(-1)^k (-2n-r-\frac{1}{2})_k}{(\frac{3}{2})_{2n+r}},$$

we obtain, summing up ${}_{2}\mathrm{F}_{1}$ at x=1 with a familiar formula (Rainville 1960, p.49),

$$\begin{split} \tilde{A}_{2m,2n} &= \sum_{r=0}^{\infty} \frac{(-\omega^2)^{m+n+r}}{4^{m+n+r-1}r!(\frac{3}{2})_{2m}(\frac{3}{2})_{2n+r}} {}_2F_1 \begin{bmatrix} -r, -2n-r-\frac{1}{2}; \\ 2m+\frac{3}{2}; \end{bmatrix} \\ &= \sum_{r=0}^{\infty} \frac{(-\omega^2)^{m+n+r}}{4^{m+n+r-1}r!(\frac{3}{2})_{2m}(\frac{3}{2})_{2n+r}} \times \frac{(\frac{3}{2})_{2m}(2m+2n+2r+1)!}{(\frac{3}{2})_{2m+r}(2m+2n+r+1)!} \\ &= \frac{4(-\omega^2)^{m+n}(\frac{3}{2})_{m+n}(m+n)!}{(\frac{3}{2})_{2m}(\frac{3}{2})_{2n}(2m+2n+1)!} {}_2F_3 \begin{bmatrix} m+n+1, m+n+\frac{3}{2}; \\ 2m+\frac{3}{2}, 2n+\frac{3}{2}, 2m+2n+2; -\omega^2 \end{bmatrix}. \end{split}$$

Likewise,

$$\begin{split} \tilde{A}_{2m+1,2n+1} &= -\frac{4(-\omega^2)^{m+n+1}(\frac{3}{2})_{m+n+1}(m+n+1)!}{(\frac{3}{2})_{2m+1}(\frac{3}{2})_{2n+1}(2m+2n+3)!} \\ &\qquad \times {}_2\mathrm{F}_3 \left[\frac{m+n+\frac{5}{2},m+n+2;}{2m+\frac{5}{2},2n+\frac{5}{2},2m+2n+4;} - \omega^2 \right]. \end{split}$$

and we deduce that for all m and n of the same parity

$$\tilde{A}_{m,n} = \frac{4(-1)^{\frac{m-n}{2}}\omega^{m+n}(\frac{3}{2})_{\frac{m+n}{2}}(\frac{m+n}{2})!}{(\frac{3}{2})_m(\frac{3}{2})_n(m+n+1)!} {}_{2}F_{3}\left[\begin{array}{c} \frac{m+n}{2}+1, \frac{m+n}{2}+\frac{3}{2};\\ m+\frac{3}{2}, n+\frac{3}{2}, m+n+2; \end{array}\right].$$
(2.11)

The explicit representation (2.11) is quite interesting for an unrelated reason. Adopting an altogether different approach, we can express $\tilde{A}_{m,n}$ is a completely different manner. Thus, let m and n be of the same parity. Then

$$\tilde{A}_{m,n} = \int_{-1}^{1} \int_{-1}^{1} P_m(x) P_n(y) (\cos \omega x \cos \omega y + \sin \omega x \sin \omega y) dx dy$$

$$\begin{split} &= \int_{-1}^{1} P_m(x) \cos \omega x \mathrm{d}x \int_{-1}^{1} P_n(x) \cos \omega x \mathrm{d}x \\ &+ \int_{-1}^{1} P_m(x) \sin \omega x \mathrm{d}x \int_{-1}^{1} P_n(x) \sin \omega x \mathrm{d}x \\ &= \begin{cases} \int_{-1}^{1} P_m(x) \cos \omega x \mathrm{d}x \int_{-1}^{1} P_n(x) \cos \omega x \mathrm{d}x, & m, n \text{ even,} \\ \int_{-1}^{1} P_m(x) \sin \omega x \mathrm{d}x \int_{-1}^{1} P_n(x) \sin \omega x \mathrm{d}x, & m, n \text{ odd.} \end{cases} \end{split}$$

Since

$$\begin{split} \int_{-1}^{1} P_{2n}(x) \cos \omega x \mathrm{d}x &= \sum_{k=0}^{\infty} \frac{(-\omega^{2})^{n+k}}{2^{2n+2k-1}k! (\frac{3}{2})_{2n+k}} = \frac{(-\omega^{2})^{n}}{2^{2n-1} (\frac{3}{2})_{2n}} {}_{0} \mathrm{F}_{1} \left[\frac{-;}{2n+\frac{3}{2};} - \frac{\omega^{2}}{4} \right] \\ &= (-1)^{n} \left(\frac{2\pi}{\omega} \right)^{\frac{1}{2}} J_{2n+\frac{1}{2}}(\omega), \\ \int_{-1}^{1} P_{2n+1}(x) \sin \omega x \mathrm{d}x &= \sum_{k=0}^{\infty} \frac{(-1)^{n+k} \omega^{2n+2k+1}}{4^{n+k}k! (\frac{3}{2})_{2n+k+1}} = \frac{(-1)^{n} \omega^{2n+1}}{4^{n} (\frac{3}{2})_{n+1}} {}_{0} \mathrm{F}_{1} \left[\frac{-;}{2n+\frac{5}{2};} - \frac{\omega^{2}}{4} \right] \\ &= (-1)^{n} \left(\frac{2\pi}{\omega} \right)^{\frac{1}{2}} J_{2n+\frac{3}{2}}(\omega), \end{split}$$

we deduce that

$$\tilde{A}_{2m,2n} = (-1)^{m+n} \frac{2\pi}{\omega} J_{2m+\frac{1}{2}}(\omega) J_{2n+\frac{1}{2}}(\omega),$$

$$\tilde{A}_{2m+1,2n+1} = (-1)^{m+n+1} \frac{2\pi}{\omega} J_{2m+\frac{3}{2}}(\omega) J_{2n+\frac{3}{2}}(\omega).$$

Comparing this with (2.11) results in a duplication formula for spherical Bessel functions.

Theorem 4 For every $m, n \in \mathbb{Z}_+$ of the same parity and all $z \in \mathbb{C}$ it is true that

$$J_{m+\frac{1}{2}}(z)J_{n+\frac{1}{2}}(z) = \frac{2z^{m+n+1}(\frac{3}{2})_{\frac{m+n}{2}}(\frac{m+n}{2})!}{\pi(\frac{3}{2})_{m}(\frac{3}{2})_{n}(m+n+1)!} {}_{2}F_{3}\left[\begin{array}{c} \frac{m+n}{2}+1, \frac{m+n}{2}+\frac{3}{2};\\ m+\frac{3}{2}, n+\frac{3}{2}, m+n+2; \end{array}\right] - z^{2}.$$
(2.12)

We have not found (2.12) in any of the usual texts on Bessel functions and believe that it might be new – a familiar situation in mathematics, when you set out to prove one thing and discover something different altogether. Note further that computer experimentation indicates that the duplication formula (2.12) is probably true for all $m, n \in \mathbb{N}$, regardless of parity. This being marginal to the theme of this paper, we did not consider this conjecture further.

Our last example in this section is the problem (1.1) with the kernel g(x,y)=xy, whose eigenfunctions have been identified in (Cochran & Hinds 1974) with angular prolate spheroidal functions. Again $\tilde{A}_{m,n}=0$ for m and n of opposite parity. Otherwise, we commence by using (2.2) to argue that for every $\lambda \in \mathbb{C}$

$$g_n(\lambda) = \int_{-1}^1 e^{\lambda y} P_n(y) dy = \sum_{k=0}^\infty \frac{\lambda^{n+2k}}{2^{n+2k-1} k! (\frac{3}{2})_{n+k}} = \frac{\lambda^n}{2^{n-1} (\frac{3}{2})_n} {}_0 F_1 \left[\frac{-}{n+\frac{3}{2}}; \frac{\lambda^2}{4} \right]$$

$$= \left(\frac{2\pi}{\lambda}\right)^{\frac{1}{2}} \mathbf{I}_{n+\frac{1}{2}}(\lambda),$$

where I_{ν} is a modified Bessel function. It follows by easy algebra on the well-known Taylor expansion of modified Bessel functions that

$$\frac{\mathrm{d}^{2k} g_{2m}(\mathrm{i}\omega y)}{\mathrm{d}y^{2k}}\Big|_{y=0} = \begin{cases} 0, & k = 0, 1, \dots, m-1, \\ 2\frac{(-1)^k k! (\frac{1}{2})_k \omega^{2k}}{(k-m)! (\frac{3}{2})_{k+m}}, & k \ge m, \end{cases}$$

$$\frac{\mathrm{d}^{2k+1}g_{2m+1}(\mathrm{i}\omega y)}{\mathrm{d}y^{2k}}\Big|_{y=0} = \begin{cases} 0, & m=0,1,\dots,m-1, \\ 2\mathrm{i}\frac{(-1)^k k!(\frac{3}{2})_k \omega^{2k+1}}{(k-m)!(\frac{3}{2})_{k+m+1}}, & k \ge m \end{cases}$$

and all other derivatives of g_n vanish. Therefore, using (2.3) again and assuming without loss of generality that $m \leq n$,

$$\begin{split} \tilde{A}_{2m,2n} &= \int_{-1}^{1} \mathrm{P}_{2n} g_{2m}(\mathrm{i}\omega y) \, \mathrm{d}y = \sum_{k=0}^{\infty} \frac{(-1)^{k+n} (k+n)! (\frac{1}{2})_{k+n} \omega^{2(k+n)}}{4^{n+k-1} k! (k+n-m)! (\frac{3}{2})_{k+m+n} (\frac{3}{2})_{2n+k}} \\ &= \frac{(-1)^n n! (\frac{1}{2})_n \omega^{2n}}{4^{n-1} (n-m)! (\frac{3}{2})_{m+n} (\frac{3}{2})_{2n}} {}_2 \mathrm{F}_3 \left[\frac{n+\frac{1}{2}, n+1;}{n-m+1, m+n+\frac{3}{2}, 2n+\frac{3}{2};} - \frac{\omega^2}{4} \right]. \end{split}$$

Similar calculation can be performed for $\tilde{A}_{2m+1,2n+1}$ and in general, for all $m \leq n, m+n$ even, we have

$$\tilde{A}_{m,n} = \frac{\lfloor \frac{n}{2} \rfloor! (\frac{1}{2})_{\lfloor \frac{n+1}{2} \rfloor} (i\omega)^n}{2^{n-1} (\frac{n-m}{2})! (\frac{3}{2})_{\frac{n+m}{2}} (\frac{3}{2})_n} {}_{2} F_{3} \left[\begin{array}{c} \lfloor \frac{n+1}{2} \rfloor + \frac{1}{2}, \lfloor \frac{n}{2} \rfloor + 1; \\ \frac{n-m}{2} + 1, \frac{n+m}{2} + \frac{3}{2}, n + \frac{3}{2}; \end{array} - \frac{\omega^2}{4} \right].$$

We will return to these examples in Section 4.

3 Expansion in trigonometric functions

A familiar alternative to expansions in orthogonal polynomials are Fourier expansions. In the current section we paint on a broader canvass, allowing more general expansions in trigonometric functions. The reason is twofold. Firstly, Fourier expansions implicitly assume periodic boundary conditions and, in their absence, result in the Gibbs effect. Secondly, they converge much too slow and represent poor choice on this score as well.

Let $\mathfrak{a} = \{a_m\}_{m \in \mathbb{Z}_+}$ and $\mathfrak{b} = \{b_m\}_{m \in \mathbb{N}}$ be two sequences of nonnegative, monotonically increasing numbers. We seek to express $f \in L[-1,1]$ in the form

$$f(x) = \sum_{m=0}^{\infty} \hat{f}_m^c \cos a_m x + \sum_{m=1}^{\infty} \hat{f}_m^s \sin b_m x.$$
 (3.1)

Density of this expansion in L[-1,1] is associated with the extension of the classical *Müntz Theorem* (Borwein & Erdélyi 1995, p.187) to the unit circle and is immediately satisfied in all cases of interest to this paper.

Expansion (3.1), in tandem with the finite section method requires orthogonality, thereby imposing further conditions on the coefficients $\mathfrak a$ and $\mathfrak b$. It is trivial to prove that this is tantamount to

$$\frac{\sin(a_m + a_n)}{a_m + a_n} + \frac{\sin(a_m - a_n)}{a_m - a_n} = \frac{\sin(b_m + b_n)}{b_m + b_n} - \frac{\sin(b_m - b_n)}{b_m - b_n} = 0$$

for all $m \neq n$. We obtain the matrix entries

$$A_{2m,2n} = \int_{-1}^{1} \int_{-1}^{1} \cos(a_m x) \cos(a_n y) K_{\omega}(x, y) \, dx \, dx, \qquad m, n \in \mathbb{Z}_+,$$

$$A_{2m,2n-1} = \int_{-1}^{1} \int_{-1}^{1} \cos(a_m x) \sin(b_n y) K_{\omega}(x, y) \, dx \, dx, \qquad m \in \mathbb{Z}_+, \ n \in \mathbb{N},$$

$$A_{2m-1,2n} = \int_{-1}^{1} \int_{-1}^{1} \sin(b_m x) \cos(a_n y) K_{\omega}(x, y) \, dx \, dx, \qquad m \in \mathbb{N}, \ n \in \mathbb{Z}_+,$$

$$A_{2m-1,2n-1} = \int_{-1}^{1} \int_{-1}^{1} \sin(b_m x) \sin(b_n y) K_{\omega}(x, y) \, dx \, dx, \qquad m, n \in \mathbb{N}.$$

3.1 Large-(m, n) asymptotics

Similarly to Section 2, we need to work out the large-(m, n) asymptotics of the $A_{m,n}$ s. The starting point to our analysis are the asymptotic expansions

$$\int_{-1}^{1} f(x) \cos(ax) dx \sim \sin a \sum_{k=0}^{\infty} \frac{(-1)^{k}}{a^{2k+1}} [f^{(2k)}(1) + f^{(2k)}(-1)]$$

$$+ \cos a \sum_{k=0}^{\infty} \frac{(-1)^{k}}{a^{2k+2}} [f^{(2k+1)}(1) - f^{(2k+1)}(-1)],$$

$$\int_{-1}^{1} f(x) \sin(bx) dx \sim -\cos b \sum_{k=0}^{\infty} \frac{(-1)^{k}}{b^{2k+1}} [f^{(2k)}(1) - f^{(2k)}(-1)]$$

$$+ \sin b \sum_{k=0}^{\infty} \frac{(-1)^{k}}{b^{2k+2}} [f^{(2k+1)}(1) + f^{(2k+1)}(-1)],$$
(3.2)

which can be easily obtained from the asymptotic expansion of $\int_{-1}^{1} f(x)e^{i\eta x} dx$ (cf. for example (Iserles & Nørsett 2005)), taking real and imaginary parts respectively.

Letting $e_i \in \{-1, 1\}, i = 2, 3, 4$, we denote

$$S_{k,l}^{[e_2,e_3,e_4]} = \partial_x^k \partial_y^l \left[K_\omega(x,y) \Big|_{x=y=1} + e_2 K_\omega(x,y) \Big|_{x=1,y=-1} + e_3 K_\omega(x,y) \Big|_{x=-1,y=1} + e_4 K_\omega(x,y) \Big|_{x=y=-1} \right].$$

Note in passing that in the important case of Abel-type kernels $K_{\omega}(x,y) = \rho(x-y)$ we have

$$\begin{split} S_{k,l}^{[1,1,1]} &= (-1)^l [2\rho^{(k+l)}(0) + \rho^{(k+l)}(2) + \rho^{(k+l)}(-2)], \\ S_{k,l}^{[-1,1,-1]} &= (-1)^l [\rho^{(k+l)}(2) - \rho^{(k+l)}(-2)], \\ S_{k,l}^{[1,-1,-1]} &= (-1)^{l+1} [\rho^{(k+l)}(2) - \rho^{(k+l)}(-2)], \\ S_{k,l}^{[-1,-1,1]} &= (-1)^l [2\rho^{(k+l)}(0) - \rho^{(k+l)}(2) - \rho^{(k+l)}(-2)]. \end{split}$$

Using (3.2) twice,

$$A_{2m,2n} \sim \sin a_m \sum_{k=0}^{\infty} \frac{(-1)^k}{a_m^{2k+1}} \int_{-1}^{1} \left[\partial_x^{2k} K_{\omega}(1,y) + \partial_x^{2k} K_{\omega}(-1,y) \right] \cos(a_n y) \, \mathrm{d}y$$

$$+ \cos a_m \sum_{k=0}^{\infty} \frac{(-1)^k}{a_m^{2k+2}} \int_{-1}^{1} \left[\partial_x^{2k+1} K_{\omega}(1,y) - \partial_x^{2k+1} K_{\omega}(-1,y) \right] \cos(a_n y) \, \mathrm{d}y$$

$$\sim \sin a_m \sin a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l}^{[1,1,1]}}{a_m^{2k+1} a_n^{2l+1}} + \sin a_m \cos a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l+1}^{[-1,1,-1]}}{a_m^{2k+1} a_n^{2l+2}}$$

$$+ \cos a_m \sin a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l}^{[1,-1,-1]}}{a_m^{2k+2} a_n^{2l+1}} + \cos a_m \cos a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l+1}^{[-1,-1,1]}}{a_m^{2k+2} a_n^{2l+2}}.$$

Likewise,

$$\begin{split} A_{2m,2n+1} &\sim -\sin a_m \cos b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l}^{[-1,1,-1]}}{a_m^{2k+1} b_n^{2l+1}} + \sin a_m \sin b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l+1}^{[1,1,1]}}{a_m^{2k+1} b_n^{2l+2}} \\ &- \cos a_m \cos b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l}^{[-1,-1,1]}}{a_m^{2k+1} b_n^{2l+2}} + \cos a_m \sin a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l+1}^{[1,-1,-1]}}{a_m^{2k+2} b_n^{2l+2}}; \\ A_{2m+1,2n} &\sim -\cos b_m \sin a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l}^{[1,-1,-1]}}{b_m^{2k+1} a_n^{2l+1}} - \cos b_m \cos a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l+1}^{[-1,-1,1]}}{b_m^{2k+2} a_n^{2l+2}} \\ &+ \sin b_m \sin a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l}^{[1,1,1]}}{b_m^{2k+2} a_n^{2l+1}} + \sin b_m \cos a_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l+1}^{[-1,1,-1]}}{b_m^{2k+2} a_n^{2l+2}}; \\ A_{2m+1,2n+1} &\sim \cos b_m \cos b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l}^{[-1,-1,1]}}{b_m^{2k+1} b_n^{2l+1}} - \cos b_m \sin b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k,2l+1}^{[1,1,1]}}{b_m^{2k+1} b_n^{2l+2}} \\ &- \sin b_m \cos b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l}^{[-1,1,-1]}}{b_m^{2k+2} b_n^{2l+1}} + \sin b_m \sin b_n \sum_{k,l=0}^{\infty} \frac{(-1)^{k+l} S_{2k+1,2l+1}^{[1,1,1]}}{b_m^{2k+2} b_n^{2l+2}}. \end{split}$$

| n | 100 | 200 | 400 | 1000 |
|---------------|--------------|--------------|--------------|--------------|
| $A_{2n,2n}$ | 3.80_02 | 5.80_{-06} | 1.59_07 | 3.39_09 |
| $A_{2n,2n+2}$ | 3.47_{-02} | 5.71_{-06} | 1.58_{-07} | 3.38_{-09} |
| $A_{2n,2n+4}$ | 2.73_{-02} | 5.61_{-06} | 1.57_{-07} | 3.37_{-09} |
| $A_{0,2n}$ | 5.50_{-04} | 1.20_{-05} | 2.34_{-06} | 3.57_{-07} |
| $A_{2,2n}$ | 5.49_{-04} | 1.18_{-05} | 2.31_{-06} | 3.52_{-07} |

Table 1: Absolute values of some $A_{m,n}$ s for the Fox–Li kernel $K_{\omega}(x,y) = e^{i\omega(x-y)^2}$ and $\omega = 100$.

Were we to make the simplest possible choice, the Fourier expansion $\mathfrak{a} = \{\pi m\}_{m \in \mathbb{Z}_+}$, $\mathfrak{b} = \{\pi n\}_{n \in \mathbb{N}}$, matrix elements would have behaved asymptotically as

$$A_{2m,2n} \sim \frac{(-1)^{m+n}}{\pi^4 m^2 n^2} S_{1,1}^{[-1,-1,1]}, \qquad A_{2m,2n+1} \sim \frac{(-1)^{m+n+1}}{\pi^3 m n^2} S_{1,0}^{[-1,-1,1]},$$

$$A_{2m+1,2n} \sim \frac{(-1)^{m+n+1}}{\pi^3 m n^2} S_{0,1}^{[-1,-1,1]}, \qquad A_{2m+1,2n+1} \sim \frac{(-1)^{m+n}}{\pi^2 m n} S_{0,0}^{[-1,-1,1]}.$$

Note in particular the disappointingly slow rate of asymptotic decay of $A_{2m+1,2n+1}$.

It makes sense to choose $\mathfrak a$ and $\mathfrak b$ so that the rate of decay of all the coefficients is as rapid as possible. It is easy to see that this goal is attained for all $K_\omega \in C^\infty([-1,1]^2)$ if and only if $\sin a_m = 0$, $\cos b_n = 0$, for $\in \mathbb Z_+$, $n \in \mathbb N$. This results in *modified Fourier expansions* (Iserles & Nørsett 2008), with $a_m = \pi m$, $b_n = \pi (n - \frac{1}{2})$. We note that this choice indeed results in an orthogonal system. Another advantage of modified Fourier expansions is that, unlike classical Fourier expansions, they converge uniformly for analytic functions, regardless of periodicity (Iserles & Nørsett 2008).

We therefore restrict ourselves in the sequel to the modified Fourier base. The large-(m,n) asymptotics are

$$A_{2m,2n} \sim (-1)^{m+n} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{\pi^{2(k+l+2)} m^{2k+2} n^{2l+2}} S_{2k+1,2l+1}^{[-1,-1,1]}, \tag{3.4}$$

$$A_{2m,2n+1} \sim (-1)^{m+n+1} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{\pi^{2(k+l+2)} m^{2k+2} (n-\frac{1}{2})^{2l+2}} S_{2k+1,2l+1}^{[1,-1,-1]}, \tag{3.5}$$

$$A_{2m+1,2n} \sim (-1)^{m+n+1} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{l+l}}{\pi^{2(k+l+2)} (m-\frac{1}{2})^{2k+2} n^{2l+2}} S_{2k+1,2l+1}^{[-1,1,-1]}, \tag{3.6}$$

$$A_{2m+1,2n+1} \sim (-1)^{m+n} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \frac{(-1)^{k+l}}{\pi^{2(k+l+2)} (m-\frac{1}{2})^{2k+2} (n-\frac{1}{2})^{2l+2}} S_{2k+1,2l+1}^{[1,1,1]}. \quad (3.7)$$

Note that (3.4)–(3.7) could have been alternatively obtained from the multivariate modified Fourier asymptotics in a cube, described in (Huybrechs et al. 2007).

In Fig. 3.1 we display absolute values of different matrix entries $A_{m,n}$ for $\omega = 100$. As clear from (3.4)–(3.7), the coefficients decay like $\mathcal{O}(n^{-4})$ when descending along diagonals, but only like $\mathcal{O}(n^{-2})$ when descending along columns (or moving rightwards along rows) of A, and this is fully reflected in the figure and in Table 1. This different rate of decay has

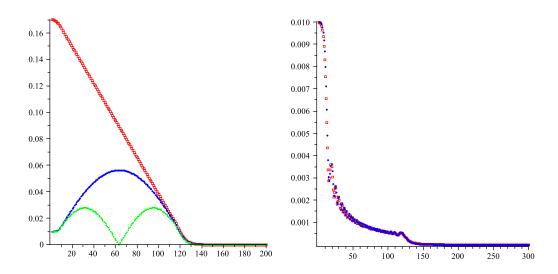


Figure 3.1: On the left, absolute values of $A_{2n,2n}$ (boxes, the straight decreasing line), $A_{2n,2n+2}$ (discs, the line with a single maximum) and $A_{2n,2n+4}$ (points, the line with two maxima) and on the right absolute values of $A_{0,2n}$ (boxes) and $A_{0,2n+1}$ (discs), all for $K_{\omega}(x,y)=\mathrm{e}^{\mathrm{i}\omega(x-y)^2}$ and $\omega=100$.

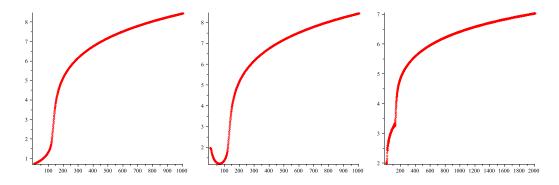


Figure 3.2: $-\log_{10}|A_{2m,2n}|$ for the Fox–Li kernel, growing n and (a) m=n; (b) m=n-2; (c) m=0, n even. In all cases $\omega=100$.

important implications, which we discuss in Section 4, to the design of effective finite section method based upon modified Fourier expansions.

Note further from Fig. 3.1 and even more from Fig. 3.2 (which should be compared with Fig. 2.1) that asymptotic large-(m,n) behaviour commences fairly rapidly, once it takes over from large- ω asymptotics. Once it happens, modified Fourier expansion converges much slower than an expansion in Legendre polynomials: sooner or later spectral convergence will beat a polynomial one. Having said so, generating the data for Fig. 3.2 was substantially

faster than the corresponding task in Fig. 2.1, although the former requires considerably more coefficients. In both instances we have used exact formulæ (which, for modified Fourier, will be introduced in the next subsection). However, an important advantage of modified Fourier becomes apparent once exact expressions for $A_{m,n}$ are not available. In the case of Legendre expansions we must resort to numerical integration, of a cost already substantial for small m and n (because of high oscillation induced by ω) and escalating rapidly when m and n grow. Modified Fourier expansions, however, can be calculated cheaply for large m and n using the asymptotic expansions (3.4)–(3.7) or their generalization to Filon-type methods in (Huybrechs et al. 2007).

Before we consider in detail the Fox–Li oscillator, we note briefly that it is possible to speed up the rate of decay of the $A_{m,n}$ by using polyharmonic bases in place of modified Fourier (Iserles & Nørsett 2006). In other words, we expand eigenfunctions in the eigenfunctions of the polyharmonic operator ∇^r in the square $[-1,1]^2$, with Neumann boundary conditions: modified Fourier expansion corresponds to r=1. In that case it is possible to show that $A_{m,n} \sim \mathcal{O}((mn)^{-r-1})$. Note that such polyharmonic orthogonal systems can be represented explicitly as linear combinations of exponentials and trigonometric functions (Iserles & Nørsett 2006).

3.2 The Fox-Li operator

Similarly to Section 2, we analyse in great detail the case $K_{\omega}(x,y) = e^{i\omega(x-y)^2}$, the Fox–Li kernel. By virtue of symmetry we have $A_{2m,2n+1} = A_{2m+1,2n} = 0$, but an explicit calculation of $A_{2m,2n}$ and $A_{2m+1,2n+1}$ is not straightforward.

Lemma 5 Let

$$\theta(a,b) = \int_{-1}^{1} \int_{-1}^{1} e^{i(ax+by)-z^2(x-y)^2} dx dy,$$

where $a, b \in \mathbb{C}$, $a + b \neq 0$ and $z \in \mathbb{C} \setminus \{0\}$ is a parameter. Then

$$\theta(a,b) = \frac{\pi^{\frac{1}{2}}}{2iz(a+b)} [F(a,b) + F(b,a)], \tag{3.8}$$

where

$$F(a,b) = \cos(a+b) \exp\left(-\frac{a^2}{4z^2}\right) \left[\operatorname{erf}\left(\frac{\mathrm{i}a}{2z} + 2z\right) + \operatorname{erf}\left(\frac{\mathrm{i}a}{2z} - 2z\right) - 2\operatorname{erf}\left(\frac{\mathrm{i}a}{2z}\right) \right] + \operatorname{i}\sin(a+b) \exp\left(-\frac{a^2}{4z^2}\right) \left[\operatorname{erf}\left(\frac{\mathrm{i}a}{2z} + 2z\right) - \operatorname{erf}\left(\frac{\mathrm{i}a}{2z} - 2z\right) \right].$$

Proof Since

$$\frac{\partial \theta}{\partial a} = \mathrm{i} \int_{-1}^{1} \int_{-1}^{1} x \mathrm{e}^{\mathrm{i}(ax+by)-z^2(x-y)^2} \, \mathrm{d}x \, \mathrm{d}y, \qquad \frac{\partial \theta}{\partial b} = \mathrm{i} \int_{-1}^{1} \int_{-1}^{1} y \mathrm{e}^{\mathrm{i}(ax+by)-z^2(x-y)^2} \, \mathrm{d}x \, \mathrm{d}y,$$

we deduce, integrating by parts, that

$$-2z^{2} \left(\frac{\partial \theta}{\partial a} - \frac{\partial \theta}{\partial b} \right) = i \int_{-1}^{1} \int_{-1}^{1} e^{i(ax+by)} \frac{de^{-z^{2}(x-y)^{2}}}{dx} dx dy$$
$$= -ia\theta(a,b) + \int_{-1}^{1} \left[e^{i(a+by)-z^{2}(1-y)^{2}} - e^{i(-a+by)-z^{2}(1+y)^{2}} \right] dy.$$

Likewise, changing the order of integration,

$$-2z^{2} \left(\frac{\partial \theta}{\partial a} - \frac{\partial \theta}{\partial b} \right) = -i \int_{-1}^{1} \int_{-1}^{1} -e^{i(ax+by)} \frac{de^{-z^{2}(x-y)^{2}}}{dy} dy dx$$
$$= ib\theta(a,b) - \int_{-1}^{1} \left[e^{i(ax+b)-z^{2}(x-y)^{2}} - -e^{i(ax-b)-z^{2}(1+x)^{2}} \right] dx.$$

We subtract the two last displayed equations from each other, whereby

$$i(a+b)\theta(a,b) = \int_{-1}^{1} \left[e^{i(a+bt)-z^2(1-t)^2} - e^{i(-a+bt)-z^2(1+t)^2} + e^{i(at+b)-z^2(1-t)^2} - e^{i(at-b)-z^2(1+t)^2} \right] dt.$$

This is an elementary integral, which we evaluate explicitly, deriving (3.8) after elementary algebra.

Corollary 1 For any $m \neq n$ it is true that

$$A_{2m,2n} = \frac{F(m\pi, n\pi) + F(n\pi, m\pi)}{4i\pi^{\frac{1}{2}}z(m+n)} + \frac{F(m\pi, -n\pi) + F(-n\pi, m\pi)}{4i\pi^{\frac{1}{2}}z(m-n)}, \quad (3.9)$$

$$A_{2m+1,2n+1} = -\frac{F((m-\frac{1}{2})\pi, (n-\frac{1}{2})\pi) + F((n-\frac{1}{2})\pi, (m-\frac{1}{2})\pi)}{4i\pi^{\frac{1}{2}}z(m+n-1)} + \frac{F((m-\frac{1}{2})\pi, -(m-\frac{1}{2})\pi) + F(-(n-\frac{1}{2})\pi, (m-\frac{1}{2})\pi)}{4i\pi^{\frac{1}{2}}z(m-n)},$$
(3.10)

where $z = (-i\omega)^{\frac{1}{2}}$.

Proof Follows at once from (3.8), because

$$A_{2m,2n} = \frac{1}{4} [\theta(m\pi, n\pi) + \theta(-m\pi, n\pi) + \theta(m\pi, -n\pi) + \theta(-m\pi, -n\pi)],$$

$$A_{2m+1,2n+1} = -\frac{1}{4} [\theta((m-\frac{1}{2})\pi, (n-\frac{1}{2})\pi) - \theta(-(m-\frac{1}{2})\pi, (n-\frac{1}{2})\pi) - \theta((m-\frac{1}{2})\pi, -(n-\frac{1}{2})\pi) + \theta(-(m-\frac{1}{2})\pi, -(n-\frac{1}{2})\pi)].$$

Since the error function is even, we have $F(a,b)+F(b,a)\equiv 0$ and the calculation simplifies.

Note that

$$F(\pi m, \pi n) = (-1)^{m+n} \exp\left(\frac{\pi^2 m^2}{4i\omega}\right) \left[\operatorname{erf}\left(\frac{i\pi m}{2(-i\omega)^{\frac{1}{2}}} + 2(-i\omega)^{\frac{1}{2}}\right) \right]$$

$$\begin{split} &+ \operatorname{erf} \left(\frac{\mathrm{i} \pi m}{2 (-\mathrm{i} \omega)^{\frac{1}{2}}} - 2 (-\mathrm{i} \omega)^{\frac{1}{2}} \right) - 2 \operatorname{erf} \left(\frac{\mathrm{i} \pi m}{2 (-\mathrm{i} \omega)^{\frac{1}{2}}} \right) \right], \\ F(\pi(m - \frac{1}{2}), \pi(n - \frac{1}{2})) &= (-1)^{m + n - 1} \exp \left(\frac{\pi^2 (m - \frac{1}{2})^2}{4 \mathrm{i} \omega} \right) \left[\operatorname{erf} \left(\frac{\mathrm{i} \pi (m - \frac{1}{2})}{2 (-\mathrm{i} \omega)^{\frac{1}{2}}} + 2 (-\mathrm{i} \omega)^{\frac{1}{2}} \right) \right. \\ &+ \left. \operatorname{erf} \left(\frac{\mathrm{i} \pi (m - \frac{1}{2})}{2 (-\mathrm{i} \omega)^{\frac{1}{2}}} - 2 (-\mathrm{i} \omega)^{\frac{1}{2}} \right) - 2 \operatorname{erf} \left(\frac{\mathrm{i} \pi (m - \frac{1}{2})}{2 (-\mathrm{i} \omega)^{\frac{1}{2}}} \right) \right], \end{split}$$

somewhat simplifying the calculations.

It remains to derive the diagonal elements $A_{n,n}$.

Lemma 6 It is true that

$$\theta(a, -a) = \frac{\pi^{\frac{1}{2}}}{z} \exp\left(-\frac{a^2}{4z^2}\right) \left[\operatorname{erf}\left(\frac{\mathrm{i}a}{2z} + 2z\right) - \operatorname{erf}\left(\frac{\mathrm{i}a}{2z} - 2z\right)\right] + \frac{\mathrm{e}^{-4z^2}\cos(2a) - 1}{z^2} + \frac{\pi^{\frac{1}{2}}\mathrm{i}a}{4z^3} \exp\left(-\frac{a^2}{4z^2}\right) \left[\operatorname{erf}\left(\frac{\mathrm{i}a}{2z} + 2z\right) + \operatorname{erf}\left(\frac{\mathrm{i}a}{2z} - 2z\right) - 2\operatorname{erf}\left(\frac{\mathrm{i}a}{2z}\right)\right].$$

Proof Changing variables and exchanging order of integration,

$$\int_{-1}^{1} \int_{-1}^{1} e^{ia(x-y)-z^2(x-y)^2} dx dy = \int_{-1}^{1} \int_{-1-y}^{1-y} e^{iat-z^2t^2} dt dy = \int_{-2}^{2} (2-|t|)e^{iat-zt^2} dt,$$

an elementary integral.

It is now trivial to express the diagonal coefficients in the form

$$A_{2n,2n} = \frac{1}{2} [\theta(\pi n, \pi n) + \theta(\pi n, -\pi n)]$$

$$A_{2n+1,2n+1} = \frac{1}{2} [\theta((n - \frac{1}{2})\pi, -(n - \frac{1}{2})\pi) - \theta((n - \frac{1}{2})\pi, (n - \frac{1}{2})\pi)],$$

both with $(-i\omega)^{\frac{1}{2}}$. Explicit expressions are long, although easy to derive, and they add little to our comprehension.

3.3 Other oscillators

The modified Fourier coefficients for the rank-2 kernel $K_{\omega}(x,y) = \cos \omega(x-y)$ can be evaluated with great ease,

$$A_{2m,2n} = \frac{4(-1)^{n+m}\omega^2 \sin^2 \omega}{(\pi^2 m^2 - \omega^2)(\pi^2 n^2 - \omega^2)},$$

$$A_{2m+1,2n+1} = \frac{4(-1)^{m+n}\omega^2 \cos^2 \omega}{[\pi^2 (m - \frac{1}{2})^2 - \omega^2][\pi^2 (n - \frac{1}{2})^2 - \omega^2]}, \quad m, n \in \mathbb{Z}_+,$$

while $A_{m,n}=0$ for odd m+n. Like in Subsection 2.4, the matrix A is of rank 2. Moreover, once we let $A_E=(A_{2m,2n})_{m,n\in\mathbb{Z}_+}$, $A_O=(A_{2m+1,2n+1})_{m,n\in\mathbb{Z}_+}$, we obtain two rank-1 matrices and in each case the nonzero eigenvalue is the sum of squares of diagonal elements. Consistently with our intention from Subsection 2.4 to use this simple example as a proving

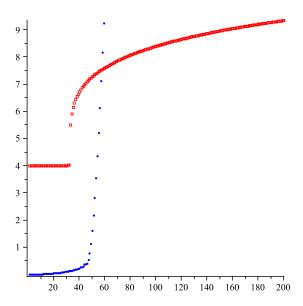


Figure 3.3: The number of significant digits in approximating one of the two nonzero eigenvalues for $K_{\omega}(x,y) = \cos \omega(x-y)$, $\omega = 100$, with an $N \times N$ matrix: squares denote modified Fourier and discs the Legendre expansion.

ground of the finite section method, we display in Fig. 3.3 the number of significant digits once the eigenvalue $1+(2\omega)^{-1}\sin 2\omega$ is approximated by $\sum_{m=1}^{N}A_{m,m}^2$ for modified Fourier and Legendre expansions and $\omega=100$.

As expected, eventually Legendre must win and, once it has overcome the influence of ω -induced oscillations, it does so with style. However, two observations demonstrate that modified Fourier expansion is not necessarily uniformly inferior. Firstly, the initial error, in the regime dominated by large- ω asymptotics, is significantly smaller with modified Fourier: we will see in Subsection 3.4 that this corresponds to a more general pattern. Secondly, even if modified Fourier expansions converge significantly slower, we can attain fairly good accuracy with small N. This is important because the cost of generating the truncated matrix $\mathcal A$ is typically much cheaper with modified Fourier expansions and, as will will see in Section 4, the size of the effective matrix that we need consider can be reduced.

Like earlier in Subsection 2.3, we next consider the kernel $K_{\omega}(x,y) = e^{i\omega xy}$. The integral

$$\theta(a,b) = \int_{-1}^{1} \int_{-1}^{1} e^{i(ax+by+\omega xy)} dx dy$$

can be computed, e.g. using symbolic software, in terms of exponential integrals:

$$\theta(a,b) = \frac{1}{\mathrm{i}\omega} \left[\mathrm{Ei}_1 \left(\frac{(a-\omega)(b+\omega)}{\mathrm{i}\omega} \right) + \mathrm{Ei}_1 \left(\frac{(a+\omega)(b-\omega)}{\mathrm{i}\omega} \right) - \mathrm{Ei}_1 \left(\frac{(a+\omega)(b+\omega)}{\mathrm{i}\omega} \right) \right]$$

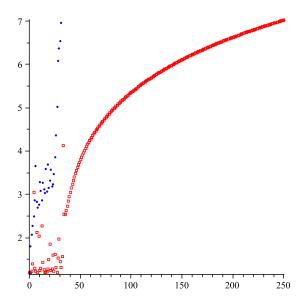


Figure 3.4: $-\log_{10} |A_{2n,2n}|$ for the kernel $K_{\omega}(x,y) = e^{i\omega xy}$ and $\omega = 100$: squares stand for modified Fourier and discs for Legendre expansions.

$$-\operatorname{Ei}_1\left(\frac{(a-\omega)(b-\omega)}{\mathrm{i}\omega}\right)\right] + \left\{\begin{array}{l} \frac{2\pi}{\omega}\exp\left(-\frac{\mathrm{i} ab}{\omega}\right), & |a|,|b| \leq \omega, \\ 0, & \text{otherwise,} \end{array}\right.$$

where Ei₁ is the exponential integral (Abramowitz & Stegun 1964, p. 227). Since $\theta(a,b) = \theta(-a,-b)$, we deduce that

$$A_{2m,2n} = \frac{1}{2} [\theta(m\pi, n\pi) + \theta(m\pi, -n\pi)],$$

$$A_{2m+1,2n+1} = \frac{1}{2} [\theta((m - \frac{1}{2})\pi, -(n - \frac{1}{2})\pi) - \theta((m - \frac{1}{2})\pi, (n - \frac{1}{2})\pi)]$$

– again, $A_{m,n} = 0$ when m + n is odd.

In Fig. 3.4 we display the number of significant digits in $A_{2n,2n}$ using modified Fourier and Legendre expansions. Evidently, up to about n=30 both expansions produce largish coefficients and then large-(m,n) asymptotics win, Legendre coefficients decay very rapidly and modified Fourier coefficients much more sedately.

3.4 Large- ω asymptotics

Let us assume for simplicity an Abel kernel of the form $K_{\omega}(x,y) = \mathrm{e}^{\mathrm{i}\omega g(x-y)}$, where $g \in \mathrm{C}^{\infty}[-2,2]$. We further assume that g is an even function, g'(0) = 0, $g''(0) \neq 0$ and that otherwise $g' \neq 0$ – this definitely represents loss of generality but the Fox–Li operator survives. Our present concern is estimate the size of the coefficients when m and n are sufficiently small and the ω -generated oscillation prevails. To this end we need to investigate

integrals of the form

$$I[f] = \int_{-1}^{1} \int_{-1}^{1} f(x, y) e^{i\omega g(x-y)} dx dy.$$
 (3.11)

Note that in our case $f(x,y) = \phi_m(x)\phi_n(y)$, but it is more convenient by this stage to work in a more general setting.

(3.11) is a bivariate highly oscillatory integral, of a kind considered in (Wong 2001) and elsewhere. Within the framework of asymptotic analysis it is exceptional, because the entire line x = y consists of stationary points, $\nabla g(x, x) = \mathbf{0}$.

Letting t = x - y, we trivially obtain

$$I[f] = \int_{-2}^{0} h^{[-]}(t)e^{i\omega g(t)} dt + \int_{0}^{2} h^{[+]}(t)e^{i\omega g(t)} dt,$$

where

$$h^{[-]}(t) = \int_{-1-t}^{1} f(t+y,y) \, \mathrm{d}y, \qquad h^{[+]}(t) = \int_{-1}^{1-t} f(t+y,y) \, \mathrm{d}y.$$

Therefore the problem reduces to two univariate integrals, of a kind that can be readily expanded for $\omega \gg 1$ using the theory in (Iserles & Nørsett 2005),

$$\int_{0}^{2} h^{[+]}(t)e^{i\omega g(t)} dt \sim -\sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[\frac{h_{m}^{[+]}(2) - h_{m}^{[+]}(0)}{g'(2)} e^{i\omega g(2)} - \frac{h_{m}^{[+]}'(0)}{g''(0)} e^{i\omega g(0)} \right]$$

$$+ \int_{0}^{2} e^{i\omega g(t)} dt \sum_{m=0}^{\infty} \frac{h_{m}^{[+]}(0)}{(-i\omega)^{m}},$$

$$\int_{-2}^{0} h^{[-]}(t)e^{i\omega g(t)} dt \sim \sum_{m=0}^{\infty} \frac{1}{(-i\omega)^{m+1}} \left[\frac{h_{m}^{[-]}(-2) - h_{m}^{[-]}(0)}{g'(-2)} e^{i\omega g(-2)} - \frac{h_{m}^{[-]}'(0)}{g''(0)} e^{i\omega g(0)} \right]$$

$$+ \int_{-2}^{0} e^{i\omega g(t)} dt \sum_{m=0}^{\infty} \frac{h_{m}^{[-]}(0)}{(-i\omega)^{m}},$$

where

$$h_0^{[\pm]}(t) = h^{[\pm]}(t), \qquad h_{m+1}^{[\pm]}(t) = \frac{\mathrm{d}}{\mathrm{d}t} \frac{h_m^{[\pm]}(t) - h_m^{[\pm]}(0)}{g'(t)}, \quad m \in \mathbb{N}.$$

Let us now consider in greater detail the case $g(x)=x^2$ of the Fox–Li operator, since it is indicative of a more general pattern of behaviour. Insofar as the modified Fourier basis is concerned, commencing from the cosine terms, we have for all m and n

$$m \neq n: \qquad h^{[-]}(t) = (-1)^{m+n} \frac{m \sin(\pi m t) - n \sin(\pi n t)}{\pi (m^2 - n^2)},$$
$$h^{[+]}(t) = -h^{[-]}(t),$$
$$m = n: \qquad h^{[-]}(t) = (1 + \frac{1}{2}t)\cos(\pi n t) + \frac{1}{2}\frac{\sin(\pi n t)}{\pi n},$$
$$h^{[+]}(t) = (1 - \frac{1}{2}t)\cos(\pi n t) - \frac{1}{2}\frac{\sin(\pi n t)}{\pi n}.$$

We examine first the off-diagonal case $m \neq n$. Easy induction confirms that

$$h_r^{[-]}(t) = (-1)^{m+n+r} \sum_{k=0}^{\infty} \frac{(-1)^k (k+1)_r}{(2k+2r)!} \frac{m^{2(k+r+1)} - n^{2(k+r+1)}}{m^2 - n^2} \pi^{2(k+r)} t^{2k+1}, \quad r \in \mathbb{Z}_+,$$

therefore $h_r^{[-]}(0) = h_r^{[+]}(0) = 0$ and

$$h_r^{[-]'}(0) = (-1)^{m+n+r+1} \pi^{2(r+1)} \frac{(r+1)!}{(2r+2)!} \frac{m^{2(r+2)} - n^{2(r+2)}}{m^2 - n^2},$$

$$h_r^{[+]'}(0) = (-1)^{m+n+r} \pi^{2(r+1)} \frac{(r+1)!}{(2r+2)!} \frac{m^{2(r+2)} - n^{2(r+2)}}{m^2 - n^2}.$$

Moreover,

$$\begin{split} h_r^{[-]}(t) &= \frac{(-1)^{m+n+r}\pi^{2r}}{4^r(\frac{1}{2})_r} \sum_{k=0}^{\infty} \frac{(-1)^k}{4^k k! (r+\frac{1}{2})_k} \frac{m^{2(k+r+1)} - n^{2(k+r+1)}}{m^2 - n^2} t^{2k+1} \\ &= \frac{(-1)^{m+n+r}\pi^{2r}t}{4^r(\frac{1}{2})_r (m^2 - n^2)} \bigg\{ m^{2(r+1)}{}_0 \mathcal{F}_1 \bigg[\frac{-;}{r+\frac{1}{2};} - \frac{(\pi m t)^2}{4} \bigg] - n^{2(r+1)}{}_0 \mathcal{F}_1 \bigg[\frac{-;}{r+\frac{1}{2};} - \frac{(\pi n t)^2}{4} \bigg] \bigg\} \\ &= \frac{(-1)^{m+n+r}\pi^{r+1}}{2^{r+\frac{1}{2}} (m^2 - n^2) t^{r-\frac{3}{2}}} \left[m^{r+\frac{3}{2}} \mathcal{J}_{r-\frac{1}{2}} (\pi m t) - n^{r+\frac{3}{2}} \mathcal{J}_{r-\frac{1}{2}} (\pi n t) \right] \\ &= \frac{(-1)^{m+n+1}\pi^{r+1}}{2^r t^{r-1} (m^2 - n^2)} [m^{r+2} \mathcal{j}_{r-1} (\pi m t) - n^{r+2} \mathcal{j}_{r-1} (\pi n t)], \end{split}$$

where j_n is the *n*th spherical Bessel function (Abramowitz & Stegun 1964, p. 437). Since

$$j_s(z) = \sin(z - \frac{\pi s}{2}) \sum_{j=0}^{\lfloor \frac{s}{2} \rfloor} \frac{(-1)^j 2^{-2j} z^{-2j-1} (s+2j)!}{(2j)! (s-2j)!}$$

$$+ \cos(z - \frac{\pi s}{2}) \sum_{j=0}^{\lfloor \frac{s-1}{2} \rfloor} \frac{(-1)^j 2^{-2j-2} z^{-2j-2} (s+1+2j)!}{(2j+1)! (s-2j-1)!}$$

(cf. http://functions.wolfram.com/03.21.03.0036.01), we obtain

$$j_{r-1}(-2\pi m) = 2(-1)^{r-1} \sum_{j=0}^{\lfloor \frac{r-1}{2} \rfloor} (-1)^j \frac{(r+2j-1)!}{(2j)!(r-2j-1)!} \frac{1}{(4\pi m)^{2j+1}}$$

and similar expression for $j_{r-1}(2\pi m)$. We observe that both values grow like $\mathcal{O}(M^{2r})$ as $r \gg 1$, where $M = \max\{m, n\}$.

This provides explicitly the values of $h_r^{[-]}$ at 0 and -2 and, similarly, of $h_r^{[+]}$ at 0 and +2. Substitution into the asymptotic expansion yields

$$A_{2m,2n} \sim \sum_{r=0}^{\infty} \frac{1}{(-i\omega)^{r+1}} \left[\frac{1}{2} h_r^{[-]}(2) e^{4i\omega} - \frac{1}{2} h_r^{[-]}(-2) e^{4i\omega} - h_r^{[-]'}(0) \right].$$
 (3.12)

It follows at once from our analysis that the asymptotic expansion (3.12) converges when $m, n < \omega^{\frac{1}{2}}$. Thus, in this regime we can use it as an effective means to calculate the entries of A.

In the remaining case m = n we have

$$h^{[-]}(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} (\pi n)^{2k} t^{2k} + \sum_{k=0}^{\infty} \frac{(-1)^k (k+1)}{(2k+1)!} (\pi n)^{2k} t^{2k+1},$$

$$h^{[+]}(t) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} (\pi n)^{2k} t^{2k} - \sum_{k=0}^{\infty} \frac{(-1)^k (k+1)}{(2k+1)!} (\pi n)^{2k} t^{2k+1}.$$

Therefore (restricting our attention to $h^{[-]}$ but noting that identical analysis applies to $h^{[+]}$)

$$h_r^{[-]}(t) = (-1)^r \sum_{k=0}^{\infty} \frac{(-1)^k (k + \frac{1}{2})_r}{(2k + 2r)!} (\pi n)^{2(k+r)} t^{2k}$$

$$+ (-1)^r \sum_{k=0}^{\infty} \frac{(-1)^k (k+1)_{r+1}}{(2k + 2r + 1)!} (\pi n)^{2(k+r)} t^{2k+1}$$

and we deduce that

$$h_r^{[-]}(0) = (-1)^r \frac{(\pi n)^{2r}}{4^r r!}, \qquad h_r^{[-]'}(0) = (-1)^r \frac{(r+1)!}{(2r+1)!} (\pi n)^{2r}.$$

To identify $h_r^{[-]}(-2)$ we compute, after much algebra,

$$\begin{split} h_r^{[-]}(t) &= \frac{(-1)^r (2\pi)^{2r}}{4^r r!} {}_1 \mathbf{F}_2 \bigg[\frac{1}{\frac{1}{2}}, r+1; \, -\frac{(\pi n t)^2}{4} \bigg] \\ &+ \frac{(-1)^r (2\pi)^{2r} (r+1) t}{2^{2r+1} (\frac{1}{2})_{r+1}} {}_1 \mathbf{F}_2 \bigg[\frac{r+2;}{r+1, r+\frac{3}{2};} \, -\frac{(\pi n t)^2}{4} \bigg]. \end{split}$$

We obtain two Bessel-like functions. (It is possible to represent the second function as a linear combination of two spherical Bessel functions, but this adds little to the narrative of this paper.)

Similar analysis extends to the odd coefficients $A_{2m+1,2n+1}$, whence

$$h^{[-]}(t) = \frac{(-1)^{m+n}}{\pi[(m-\frac{1}{2})^2 - (n-\frac{1}{2})^2]}[(m-\frac{1}{2})\sin\pi(m-\frac{1}{2})t - (n-\frac{1}{2})\sin\pi(n-\frac{1}{2})t],$$

except that the formulæ become (even more) complicated.

Asymptotic expansions and algorithms based upon them (e.g. Filon-type quadrature) are often used as a very effective means to compute highly oscillatory integrals (Iserles & Nørsett 2005). This is the moment to emphasize that this is not the case in the computation of the $A_{m,n}$. The overwhelming reason is that, while large- ω asymptotics are valid when ω is substantially small than m and n and we can use large-(m,n) asymptotics when m and n are very large in comparison to ω , neither formula is of much use in the *intermediate asymptotics* regime. Thus, in Subsection 3.6 we recommend using FFT for an efficient computation of the $A_{m,n}$ s.

3.5 Large-n asymptotics

For completeness we are also interested in estimating the size of $A_{m,n}$ when n is large (that is, $\mathcal{O}(\omega)$ or larger), while m is relatively small. In other words, $0 \le m \le M$ (where M has been defined above), while $M+1 \le n \le M+1+N$ for some (large) N.

Letting

$$\sigma_m(y) = \int_{-1}^1 \cos \pi m x K_{\omega}(x, y) \, \mathrm{d}x,$$

and employing the asymptotic expansion (3.2), we have

$$A_{2m,2n} = \int_{-1}^{1} \sigma_m(y) \cos \pi ny \, dy$$

$$\sim (-1)^n \sum_{k=0}^{\infty} \frac{(-1)^k}{(\pi n)^{2k+2}} [\sigma_m^{(2k+1)}(1) - \sigma_m^{(2k+1)}(-1)]. \tag{3.13}$$

In the case of an Abel kernel $K_{\omega}(x,y)=K_{\omega}(x-y)$ we can easily demonstrate, integrating by parts, that

$$\sigma'_m(y) = -[K_\omega(1-y) - (-1)^m K_\omega(1+y)] - \pi m \int_{-1}^1 \sin \pi m x K_\omega(x-y) \, \mathrm{d}x,$$

$$\sigma''_m(y) = K'_\omega(1-y) + (-1)^m K'_\omega(1+y) - (\pi m)^2 \sigma_m(y).$$

In particular, if $K_{\omega}(y) = \mathrm{e}^{\mathrm{i}\omega g(y)}$ then $\sigma'_m(y)$ scales like $m, \sigma''_m(y)$ like $\max\{\omega, m^2\}$ and it is easy to prove that, in general, $\sigma^{(k)}_m$ scales like $\max\{\omega^{k-1}, m^k\}$. Given that within our regime $n > m, \omega$, it thus follows from (3.13) that the asymptotic expansion is convergent at a geometric speed.

3.6 Computation of the modified Fourier matrix

Given suitably large $s \in \mathbb{N}$, we wish to compute $A_{m,n}$ for $m,n=0,1,\ldots,s-1$ and the modified Fourier basis. The simplest approach is also probably the most effective for a general kernel K_{ω} , namely to compute

$$A_{2m,2n} = \int_{-1}^{1} \int_{-1}^{1} \cos(\pi m x) \cos(\pi n y) K_{\omega}(x, y) \, \mathrm{d}x \, \mathrm{d}y,$$

$$A_{2m+1,2n} = \int_{-1}^{1} \int_{-1}^{1} \sin(\pi (m - \frac{1}{2})x) \cos(\pi n y) K_{\omega}(x, y) \, \mathrm{d}x \, \mathrm{d}y,$$

$$A_{2m,2n+1} = \int_{-1}^{1} \int_{-1}^{1} \cos(\pi m x) \sin(\pi (n - \frac{1}{2})y) K_{\omega}(x, y) \, \mathrm{d}x \, \mathrm{d}y,$$

$$A_{2m+1,2n+1} = \int_{-1}^{1} \int_{-1}^{1} \sin(\pi (m - \frac{1}{2})x) \sin(\pi (n - \frac{1}{2})y) K_{\omega}(x, y) \, \mathrm{d}x \, \mathrm{d}y$$

for $m, n = 0, 1, ..., \lfloor s/2 \rfloor - 1$ using bivariate Fast Fourier Transform (FFT). Of course, s must be large enough, at least $\mathcal{O}(\omega)$, so that oscillation due to ω is not a problem, and it

helps FFT if it is a highly composite integer. The computational expense consists thus of two components. Firstly, we need to compute K_{ω} at $2s^2$ points to implement the requisite fast cosine and sine transforms, secondly we incur $\mathcal{O}(s^2 \log s)$ flops in the computation of the transforms.

Matters are considerably simpler for the Abel kernel $K_{\omega}(x,y) = \mathrm{e}^{\mathrm{i}\omega g(x-y)}$, which we have already encountered in Subsection 3.4, and like there subject to the additional conditions that g is even (hence $A_{2m+1,2n} = A_{2m,2n+1} = 0$ and need not be computed), g'(0) = 0 is the only stationary point of g in [-1,1] and $g''(0) \neq 0$. We have proved there that

$$A_{2m,2n} = \int_{-2}^{0} h_{m,n}^{[c,-]}(t) e^{i\omega g(t)} dt + \int_{0}^{2} h_{m,n}^{[c,+]}(t) e^{i\omega g(t)} dt,$$
 (3.14)

$$A_{2m+1,2n+1} = \int_{-2}^{0} h_{m,n}^{[s,-]}(t) e^{i\omega g(t)} dt + \int_{0}^{2} h_{m,n}^{[s,+]}(t) e^{i\omega g(t)} dt,$$
 (3.15)

where

$$h_{m,n}^{[c,-]}(t) = \begin{cases} (1 + \frac{1}{2}t)\cos(\pi nt) + \frac{1}{2}\frac{\sin(\pi nt)}{\pi n}, & m = n, \\ (-1)^{m+n}\frac{m\sin(\pi mt) - n\sin(\pi nt)}{\pi(m^2 - n^2)}, & m \neq n; \end{cases}$$

$$h_{m,n}^{[c,+]}(t) = \begin{cases} (1 - \frac{1}{2}t)\cos(\pi nt) - \frac{1}{2}\frac{\sin(\pi nt)}{\pi n}, & m = n, \\ (-1)^{m+n+1}\frac{m\sin(\pi mt) - n\sin(\pi nt)}{\pi(m^2 - n^2)}, & m \neq n; \end{cases}$$

$$h_{m,n}^{[s,-]}(t) = \begin{cases} (1 + \frac{1}{2}t)\cos(\pi(n - \frac{1}{2})t) + \frac{\sin(\pi(n - \frac{1}{2})t)}{\pi(2n - 1)}, & m = n, \\ (-1)^{m+n}\frac{(m - \frac{1}{2})\sin(\pi(m - \frac{1}{2})t) - (n - \frac{1}{2})\sin(\pi(n - \frac{1}{2})t)}{\pi[(m - \frac{1}{2})^2 - (n - \frac{1}{2})^2]}, & m \neq n, \end{cases}$$

$$h_{m,n}^{[s,+]}(t) = \begin{cases} (1 - \frac{1}{2}t)\cos(\pi(n - \frac{1}{2})t) - \frac{\sin(\pi(n - \frac{1}{2})t)}{\pi(2n - 1)}, & m = n, \\ (-1)^{m+n+1}\frac{(m - \frac{1}{2})\sin(\pi(m - \frac{1}{2})t) - (n - \frac{1}{2})\sin(\pi(n - \frac{1}{2})t)}{\pi[(m - \frac{1}{2})^2 - (n - \frac{1}{2})^2]}, & m \neq n. \end{cases}$$

Therefore, changing variables in a completely transparent manner, both (3.14) and (3.15) reduce to the calculation of integrals of the form

$$\begin{split} & \int_0^2 \mathrm{e}^{\mathrm{i}\omega g(t)} \sin(\pi n t) \, \mathrm{d}t, \int_0^2 \mathrm{e}^{\mathrm{i}\omega g(t)} (1 - \tfrac{1}{2} t) \cos(\pi n t) \, \mathrm{d}t, \\ & \int_0^2 \mathrm{e}^{\mathrm{i}\omega g(t)} \sin(\pi (n - \tfrac{1}{2}) t) \, \mathrm{d}t, \int_0^2 \mathrm{e}^{\mathrm{i}\omega g(t)} (1 - \tfrac{1}{2} t) \cos(\pi (n - \tfrac{1}{2}) t) \, \mathrm{d}t, \end{split}$$

and this can be accomplished with *univariate* FFTs. Thus, the cost reduces to 2s calculations of q and $\mathcal{O}(s \log s)$ flops to evaluate the discrete sine and cosine transforms.

4 The hyperbolic cross

The modified Fourier basis comes into its own as a mean to compute spectra of highly oscillatory Fourier operators once we take into account the specific rate of decay of the coefficients $A_{m,n}$ for large m and n. This is demonstrated in Fig. 4.1, where we display the values of $|A_{2m,2n}|$ (on the left) and $|A_{2m+1,2n+1}|$ (on the right) for the Fox–Li equation, $m,n \leq 800$ and $\omega = 100$. The meaning of the differently-shaded regions is as follows. The white area on bottom right corresponds to terms which are less than 10^{-7} in modulus, the adjoining light-shaded area corresponds to $10^{-7} \leq |A_{m,n}| < 10^{-6}$, the next one to $10^{-6} \leq |A_{m,n}| < 10^{-5}$ and so on. Finally, the thin diagonal sliver at top left consists of all (m,n) such that $|A_{m,n}| \geq 10^{-2}$.

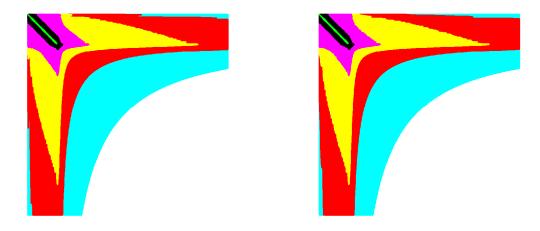


Figure 4.1: The hyperbolic cross associated with modified Fourier expansions for the Fox–Li equation, with $\omega=100$.

The pattern discernable in Fig. 4.1 is the familiar *hyperbolic cross*, originally introduced by Babenko (1960) in the context of multivariate Fourier expansions. As we already know from Subsection 3.1, using a modified Fourier basis results in

$$A_{m,n} \sim \mathcal{O}((mn)^{-2}), \quad m, n \gg 1.$$

This implies that the coefficients decay at a different rate along different directions in the matrix: fastest along diagonals and considerably slower along rows and columns. (Cf. also Fig. 3.1.) This is precisely the phenomenon visible in Fig. 4.1. Formally, let $\mathcal{A} = (A_{k,l})_{k,l \in \mathbb{Z}_+}$ be the matrix whose eigenvalues we seek. It follows that \mathcal{A} partitions into

$$\mathcal{A} = \begin{bmatrix} \mathcal{A}_{1,1} & \mathcal{A}_{1,2} \\ \mathcal{A}_{2,1} & \mathcal{A}_{2,2} \end{bmatrix}, \tag{4.1}$$

where $A_{1,1}$ is an $r \times r$ matrix, with sufficiently large r (in practice $r = \mathcal{O}(\omega)$), while the

elements of the infinite matrix $A_{2,2}$ are adequately small.¹ Let us replace the 'small' matrix $A_{2,2}$ by zero,

$$\tilde{\mathcal{A}} = \left[\begin{array}{cc} \mathcal{A}_{1,1} & \mathcal{A}_{1,2} \\ \mathcal{A}_{2,1} & O \end{array} \right].$$

The main idea is to replace the computation of $\sigma(\mathcal{A})$ by that of $\sigma(\tilde{A})$: as it turns out, the latter is a considerably simpler problem. We do not consider here the question of the distance between the two sets, while remarking that computational experience is that it is very small indeed, provided that r is large enough. Intuitively speaking, provided that $\max_{i,j\geq r+1}|A_{m,n}|$ is small, so should be the Hausdorff distance $\operatorname{dist}[\sigma(\tilde{\mathcal{A}}) - \sigma(\mathcal{A})]$, but the veracity of this statement depends on the structure of the pseudoeigenvalues of \mathcal{A} (Trefethen & Embree 2005).

Theorem 7 The matrix $\tilde{\mathcal{A}}$ is of rank 2r. Moreover, let $\mathcal{G} = \mathcal{A}_{1,2}\mathcal{A}_{2,1}$ and let \mathcal{G}_1 and \mathcal{G}_2 be any $r \times r$ matrices such that $\mathcal{G}_1\mathcal{G}_2 = \mathcal{G}$. Then the nonzero eigenvalues of $\tilde{\mathcal{A}}$ coincide with those of the $(2r) \times (2r)$ matrix

$$\mathcal{B} = \left[egin{array}{cc} \mathcal{A}_{1,1} & \mathcal{G}_1 \\ \mathcal{G}_2 & O \end{array}
ight].$$

Proof Let $\lambda \in \sigma(\tilde{A})$ and assume that $\lambda \neq 0$. Further, suppose that

$$oldsymbol{v} = \left[egin{array}{c} oldsymbol{v}_1 \ oldsymbol{v}_2 \end{array}
ight]$$

be a corresponding nonzero eigenvector, where $v_1 \in \mathbb{C}^r$. Therefore,

$$A_{1,1}v_1 + A_{1,2}v_2 = \lambda v_1, \qquad A_{2,1}v_1 = \lambda v_2.$$

We substitute $v_2 = \lambda^{-1} \mathcal{A}_{2,1} v_1$ into the first equation and multiply by $\lambda \neq 0$. The outcome is

$$(A_{12}A_{21} + \lambda A_{11} - \lambda^2 I)v_1 = 0. (4.2)$$

We therefore deduce that nonzero eigenvalues of $\tilde{\mathcal{A}}$ coincide with the solutions of (4.2), hence with the *quadratic eigenvalue problem* with the pencil $(\mathcal{G}, \mathcal{A}_{1,1}, -I)$. Since the underlying matrices are $r \times r$, the quadratic eigenvalue problem has 2r solutions and we deduce that $\mathrm{rank}\tilde{\mathcal{A}} = 2r$.

To prove the second part of the theorem, we let $\mu \in \sigma(\mathcal{B})$, $\mu \neq 0$, with a nonzero eigenvector

$$oldsymbol{u} = \left[egin{array}{c} oldsymbol{u}_1 \ oldsymbol{u}_2 \end{array}
ight], \qquad oldsymbol{u}_1, oldsymbol{u}_2 \in \mathbb{C}^r.$$

Therefore

$$A_{1,1}u_1 + G_1u_2 = \mu u_1, \qquad G_2u_1 = \mu u_2.$$

In the important case when $A_{m,n} \equiv 0$ for $m+n=1 \mod 2$, we can split $\mathcal A$ into two infinite matrices, $\mathcal A^e = (A_{2m,2n})_{m,n\in\mathbb Z_+}$ and $\mathcal A^o = (A_{2m+1,2n+1})_{m,n\in\mathbb Z_+}$, say: the Fox–Li equation is an important example. In that case both $\mathcal A^e$ and $\mathcal A^o$ can be subjected to partition (4.1) and an identical argument applies.

²The pseudospectrum of \mathcal{A} for the Fox–Li operator has been already considered in (Landau 1977/78).

As before, we substitute $u_2 = \mu^{-1} \mathcal{G}_2 u_1$ into the first equation. The outcome is

$$(\mathcal{G}_1\mathcal{G}_2 + \mu \mathcal{A}_{1,1} - \mu^2 I)u_1 = (\mathcal{G} + \mu \mathcal{A}_{1,1} - \mu^2 I)u_1 = \mathbf{0}$$

and we obtain *exactly* the same quadratic eigenvalue problem (4.2) as before. (Indeed, even the eigenvectors are the same!) It is trivial to prove that this argument works in reverse, i.e. that every solution of the quadratic eigenvalue problem yields an eigenvalue/eigenvector pair for \mathcal{B} , simply repeating the argument in reverse. This completes the proof of the theorem.

The significance of the last theorem to the computation of eigenvalues of the Fredholm problem (1.1) is clear: it suffices to choose suitably large r, form the matrix $\mathcal{A}_{1,1}$, approximate the matrix \mathcal{G} by suitably truncating the matrices $\mathcal{A}_{1,2}$ and $\mathcal{A}_{2,1}$ (i.e., calculating $A_{m,n}$ for $0 \le m, n \le s-1$, $\min\{m,n\} \le r-1$ for sufficiently large s) and compute the 2r eigenvalues of \mathcal{B} . Recall that, the operator (1.1) being compact, the eigenvalues of \mathcal{A} accumulate at the origin. In effect, what we are doing here is to set all the eigenvalues, except for the first 2r, to zero. Given that these eigenvalues are likely to be tiny, well underneath the machine epsilon of any practical computer, this procedure incurs very small error.

There are several obvious choices of \mathcal{G}_1 and \mathcal{G}_2 such that $\mathcal{G}=\mathcal{G}_1\mathcal{G}_2$. The most obvious is $\mathcal{G}_1=\mathcal{G},\,\mathcal{G}_2=I$. Another is letting $\mathcal{G}_1\mathcal{G}_2$ be the QR factorization of \mathcal{G} . An intriguing possibility in the symmetric case $\mathcal{G}_2=\mathcal{G}_1^{\top}$ is to take $\mathcal{G}_2^{\top}\mathcal{G}_2$ as the Cholesky factorization of \mathcal{G} , whereby $\mathcal{G}_1=\mathcal{G}_2^{\top}$. This has the advantage of replacing a complex symmetric infinite matrix by a complex symmetric finite one. A word of warning, however: since \mathcal{G} is complex, the existence of Cholesky factorization is not guaranteed.

Two questions remain. Firstly, is similar behaviour, namely that enough entries of $\mathcal A$ become rapidly small, in a manner that can be exploited in practical computation, extends to Legendre expansions. Fig. 4.2, where we display the size of terms in a 250×250 matrix, demonstrates that this is not so. The white shading in the bottom-right corner corresponds to $|A_{m,n}| < 10^{-20}$ and subsequent bands of colour to increase in modulus by a factor of 10^3 .

A reasonable choice of r for a modified Fourier basis with $\omega=100$ is 125 and the size of \mathcal{B} is $(2r)\times(2r)$. On the face of it, whether we use modified Fourier expansions or Legendre expansions, we end up with a matrix of similar size. This, however, disregards the computation of the matrix in question! According to Section 3, for general kernels the cost of computing \mathcal{A} for modified Fourier is $\mathcal{O}(s^2\log s)$ operations, to which we need to add $\mathcal{O}(r^2s)$ operations to compute $\mathcal{G}=\mathcal{A}_{1,2}\mathcal{A}_{2,1}$. In the case of an Abel kernel the cost of computing \mathcal{A} is just $\mathcal{O}(s\log s)$ originating in FFT and $\mathcal{O}(N)$ to form N terms. Since we need to form just r^2+2rs nonzero terms of $\tilde{\mathcal{A}}$ and $s\gg r$, this means that in that case the total cost is $\mathcal{O}((r+\log s)s)$. Additional savings, which we disregard here, occur in the complex-symmetric case.

For Legendre expansion, however, there is no good way of computing the $A_{m,n}$ s. Even in special cases (e.g. the Fox–Li kernel) when we can represent the $A_{m,n}$ s explicitly as generalized hypergeometric functions, their computation is fairly expensive. Thus, while the ultimate size of matrices is similar, the cost of forming their entries is greatly smaller for the modified Fourier expansion.

The second question is whether the state of affairs demonstrated in Fig. 4.1 remains valid for other kernels. Clearly, this is so as long as K_{ω} is sufficiently smooth, so that the asymptotic estimate $A_{m,n} = \mathcal{O}((mn)^{-2})$ holds. It breaks down for kernels with derivative discontinuities

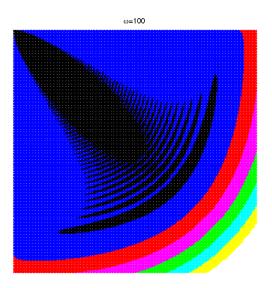


Figure 4.2: The size of the elements of $A_{m,n}$ in the Legendre expansion for the Fox–Li operator with $\omega=100$.

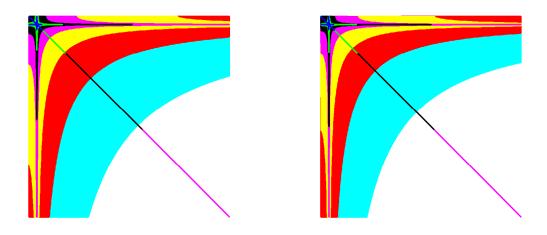


Figure 4.3: The size of the elements $A_{2m,2n}$ and $A_{2m+1,2n+1}$ for $K_{\omega}(x,y)=\mathrm{e}^{\mathrm{i}\omega|x-y|}$ and $\omega=100$ using modified Fourier basis and $m,n=0,1,\ldots,800$.

As an example of such breakdown, we consider in Fig. 4.3 the kernel $K_{\omega}(x,y) = \mathrm{e}^{\mathrm{i}\omega|x-y|}$. It is easy to evaluate the coefficients in a modified Fourier expansion explicitly. Thus, $A_{m,n} = 0$ for $m+n=1 \mod 2$ and (assuming that ω is not an integer multiple of π)

$$A_{2m,2n} = \begin{cases} \frac{2i\omega[\omega^2 - i\omega(1 - e^{2i\omega}) - \pi^2 m^2]}{(\omega^2 - \pi^2 m^2)^2}, & m = n, \\ \frac{2(-1)^{m+n}\omega^2(1 - e^{2i\omega})}{(\omega^2 - \pi^2 m^2)(\omega^2 - \pi^2 n^2)}, & m \neq n; \end{cases}$$

$$A_{2m+1,2n+1} = \begin{cases} \frac{2i\omega[\omega^2 - i\omega(1 + e^{2i\omega}) - \pi^2(m - \frac{1}{2})^2]}{[\omega^2 - \pi^2(m - \frac{1}{2})^2]^2}, & m = n, \\ \frac{2(-1)^{m+n}\omega^2(1 + e^{2i\omega})}{[\omega^2 - \pi^2(m - \frac{1}{2})^2][\omega^2 - \pi^2(n - \frac{1}{2})^2]}, & m \neq n. \end{cases}$$

In Fig. 4.3 we display the size of the 'even' and 'odd' coefficients $A_{m,n}$ for the modified Fourier basis. Evidently, the entries exhibit a hyperbolic cross, except for diagonal elements, which decay like $\mathcal{O}(n^{-2})$, a consequence of derivative discontinuity in K_{ω} . Note that the spectrum in this case has been derived (as an asymptotic expansion in ω^{-1}) in (Brunner et al. 2008), hence we do not require the finite section method to this end.

5 Conclusions

Spectral problems for highly oscillatory Fredholm kernels are important, not least because of their relevance to laser dynamics, and they are exceedingly challenging from mathematical and numerical points of view. In this paper we continue the project on which we have embarked in (Brunner et al. 2008), to shed light on such problems. Specifically, we have considered the method of finite section, a natural approach toward the evaluation of the spectrum.

The obvious choice of basis in finite section method is Legendre polynomials, because of their very rapid convergence. However, the onset of this rapid convergence is only after oscillations due to the kernel have been resolved, hence the outcome is a matrix which is not small. Worse, there are simply no good methods to evaluate matrix coefficients, double integrals involving Legendre polynomials, efficiently.

An alternative to Legendre polynomials is to use a modified Fourier basis. On the face of it, the convergence rate is considerably slower, $\mathcal{O}((mn)^{-2})$ compared to spectral. Yet, implemented by exploiting the hyperbolic cross structure, they result in matrices not much greater than those originating in the Legendre basis, but whose coefficients can be calculated very rapidly with FFT.

Is modified Fourier expansion more efficient than Legendre? This in large measure depends on the values of ω : the higher the oscillation, the greater the likelihood of modified Fourier prevailing. However, a resolution of this question calls for fine-tuning of a wide range of parameters and implementation options, as well as a great deal of numerical experimentation for different kernels and values of ω , beyond the scope of the current paper.

Numerous challenges remain in the understanding of highly oscillatory Fredholm spectral problems. The most fascinating to our mind is the mathematical structure of the Fox–Li spectrum. We have plotted the spectrum for $\omega=100$ (as obtained with the finite section method, using modified Fourier basis with r=127 and s=800) in Fig. 5.1. Similar information is

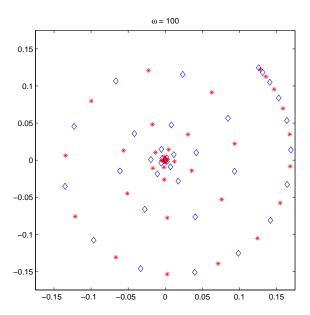


Figure 5.1: The eigenvalues of the Fox–Li operator for $\omega=100$. The diamonds correspond to 'even' eigenvalues (that is, following from expansion in cosines) and stars to 'odd' eigenvalues.

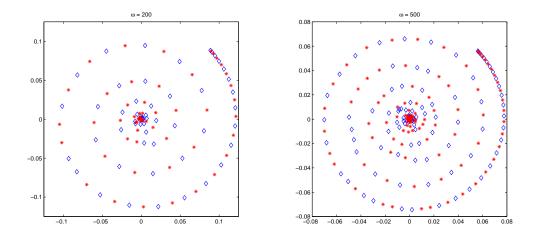


Figure 5.2: The same as Fig. 5.1, except for $\omega=200$ (on the left) and $\omega=500$.

presented in Fig. 5.2 for $\omega=200$ and $\omega=500$. Evidently, the eigenvalues lie on a spiral. What is this spiral? How does it vary with ω ?

Of course, even understanding of the structure of the Fox-Li spectrum is but a first step on a longer journey into the unknown: understanding the spectra of general Fredholm problems with high oscillation. The work of this paper, as well as (Brunner et al. 2008), need be seen as first and hesitant steps toward this goal.

We have plotted the eigenfunctions corresponding to some eigenvalues in Fig. 5.3, and again it is striking how much structure can be observed. Clearly, for small values of n (that is, for eigenvalues near the outer arm of the spiral) the eigenfunctions are perturbed trigonometric functions, while for large n they are (perturbed?) wave packets. Note that changing variables $x \to x/\sqrt{\omega}$, $y \to y/\sqrt{\omega}$, $\lambda \to \lambda/\sqrt{\omega}$ results in the spectral problem

$$\int_{-\sqrt{\omega}}^{\sqrt{\omega}} f(x) e^{i(x-y)^2} dx = \lambda f(y), \qquad -\sqrt{\omega} \le y \le \sqrt{\omega}.$$

Now, were we to replace the interval of integration by the real line, i.e. consider the problem

$$\int_{-\infty}^{\infty} f(x)e^{i(x-y)^2} dx = \lambda f(y), \quad -\infty < y < \infty,$$

we would have recovered a spectrum of a Schrödinger operator which, indeed, possesses the above features: 'low' eigenfunctions resemble trigonometric functions, 'high' eigenfunctions are wave packets.³ Yet, what is the discrepancy between the two problems? Can we infer the first from the second?

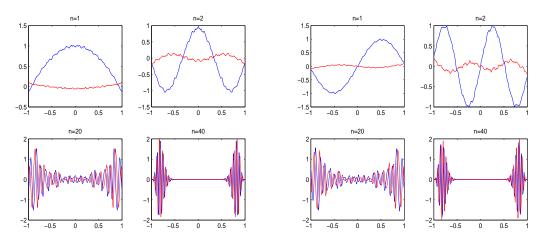


Figure 5.3: Real and imaginary parts of the eigenfunctions corresponding to the first, second, twentieth and fortieth 'even' and 'odd' eigenvalues, respectively, for $\omega = 100$.

Much remains to be done to understand highly oscillatory Fredholm problems. We hope that this paper contributes in some measure toward this goal.

³We are grateful to Olof Runborg for this observation.

Acknowledgements

Much of the research leading toward this paper has been done during the "Highly oscillatory problems" programme at the Isaac Newton Institute of Mathematical Sciences in Cambridge in Winter–Spring 2007. The authors are grateful to the staff of the institute for superb research conditions and to participants of the programme for many illuminating discussions. They would also like to acknowledge useful discussions with a number of colleagues, in particular Ben Adcock (Cambridge), Michael Berry (Bristol), Alfredo Deaño (Cambridge), Percy Deift (NYU), Alexander Its (Indiana), Allan Pinkus (Technion), Einar Rønquist (NTNU Trondheim) and Olof Runborg (KTH Stockholm). We wish also to acknowledge the insightful and well-informed comments of the two referees.

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