On the numerical quadrature of highly-oscillating integrals I: Fourier transforms

Arieh Iserles*

June 6, 2003

Abstract

Highly-oscillatory integrals are allegedly difficult to calculate. The main assertion of this paper is that impression is incorrect. As long as appropriate quadrature methods are used, their accuracy *increases* when oscillation becomes faster and suitable choice of quadrature points renders this welcome phenomenon more pronounced. We focus our analysis on *Filon-type quadrature* and analyse its behaviour in a range of frequency regimes for integrals of the form $\int_0^h f(x)\mathrm{e}^{\mathrm{i}\omega x}w(x)\,\mathrm{d}x$, where $h > 0$ is small and $|\omega|$ large.

Our analysis is applied to modified Magnus methods for highly-oscillatory ordinary differential equations.

1 Introduction

The computation of integrals of highly-oscillating functions is one of the oldest and, arguably, most important issues in numerical analysis. Highly-oscillating integrals abound in applications, from electromagnetics to quantum physics and chemistry, fluid mechanics, molecular dynamics, ... Methods have existed for a long while and, indeed, the most fruitful idea (as we hope to persuade the reader) has been published three quarters of a century ago (Filon 1928) and, in a more modern guise, half a century ago (Luke 1954). Yet, it is difficult to identify any other area of scientific computing equally plagued by vague assertions, false "folk wisdom" and plainly misleading statements.

The subject matter of this paper is the computation of

$$I_h[f] = \int_0^h f(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x, \tag{1.1}$$

where $h > 0$ is small, while $\omega \in \mathbb{R}$ is such that $|\omega| \gg 1$: typically, the *characteristic frequency* $h\omega$ of (1.1) is large. Note that ω need not be an integer multiple of $2\pi/h$, therefore (1.1) is, strictly speaking, a more general construct than a Fourier transform. Having said this, the computation of a single Fourier transform of a given function is probably the most ubiquitous application, and this is reflected in the title of this paper.

*Department of Applied Mathematics and Theoretical Physics, Centre for Mathematical Sciences, Wilberforce Rd, Cambridge CB3 0WA, United Kingdom, email ai@damtp.cam.ac.uk.

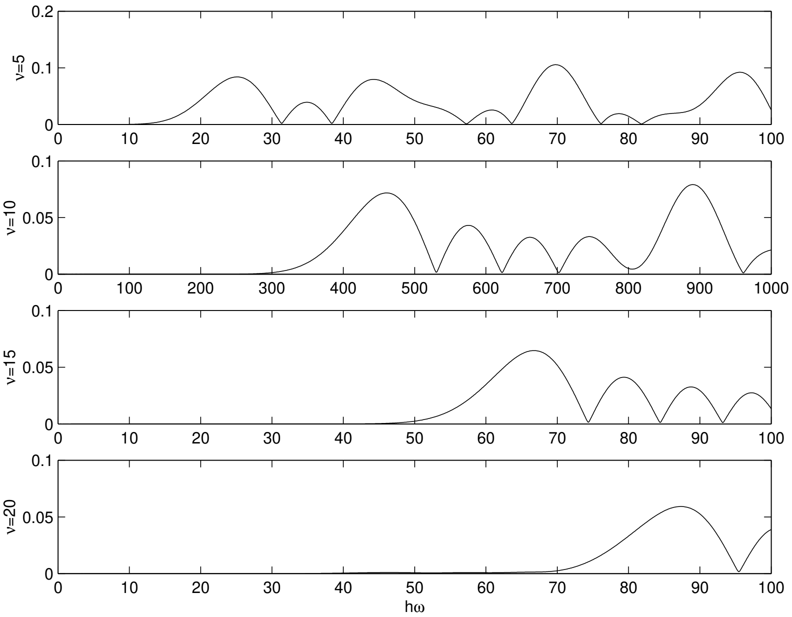

Figure 1: The error in Gauss–Legendre integration of (1.1) for $f(x) = \mathrm{e}^x$, $h = \frac{1}{10}$ and different values of ω.

Numerical integration is a mature, well-understood subject, there are many clear and comprehensive monographs devoted to this area of activity, in particular (Davis & Rabinowitz 1980) and (Engels 1980), and it might seem that the task is straightforward, more appropriate for elementary courses in numerical computation than for research papers. The natural candidate for a good computational method, indeed the method of choice for numerical integration, is the *Gauss–Christoffel quadrature*

$$Q_h^{\mathrm{GC}}[f] = h \sum_{l=1}^{\nu} b_l f(c_l h) \mathrm{e}^{\mathrm{i}\omega c_l h}, \tag{1.2}$$

where $c_1, c_2, \ldots, c_\nu \in [0,1]$ are distinct nodes, while $b_1, b_2, \ldots, b_\nu$ are interpolatory weights (Gautschi 1981). The order of (1.2) is determined by orthogonality conditions and, in particular, if $c_1, c_2, \ldots, c_\nu$ are selected as the zeros of the νth Legendre polynomial, shifted to the interval $[0,1]$, then the quadrature is of order 2ν (i.e., exact for all $f \in \mathbb{P}_{2\nu-1}$ or, in other words, bearing the error of $\mathcal{O}\big(h^{2\nu+1}\big)$ for $h \to 0$). No other method can exceed the order of Gauss–Legendre quadrature, hence this is a good point of departure for our discussion. Thus, Figure 1 displays the absolute error in the integration of (1.1) with $f(x) = \mathrm{e}^x$ by Gauss–Legendre schemes with $\nu \in \{5, 10, 15, 20\}$ and $h = \frac{1}{10}$, for characteristic frequency $h\omega \in [0, 100]$. While, unsurprisingly, the methods do well for small $h\omega$, the error in the higher range of frequencies is unacceptably large. Moreover, it is hardly attenuated when the number of quadrature points increases.

The reason for the failure of Gauss–Legendre quadrature, indeed of *any* Gauss–Christoffel quadrature (1.2), is obvious. The exact integral in Fig. 1 is $(\mathrm{e}^{(1+\mathrm{i}\omega)h} - 1)/(1 + \mathrm{i}\omega)$ and its envelope attenuates like $\mathcal{O}(\omega^{-1})$ for $\omega \gg 1$. This is nothing but an illustration of the well-known Riemann–Lebesgue lemma: for every $f \in \mathrm{L}_2[0, h]$ it is true that $\lim_{\omega\to\infty} I_h[f] = 0$. There is, though, absolutely no reason why the *finite* combination (1.2) of function values should tend to zero as $\omega \to \infty$. Convergence of Gauss–Christoffel makes sense only if ω is kept constant while $h \to 0$, but then the characteristic frequency tends to zero as well and the system is not highly oscillatory any more.

As an aside, ergodic theory tells us that convergence of Gauss–Christoffel occurs also when ω and h are kept constant while $\nu \to \infty$. Indeed, if f is h-periodic and the c_ls are equidistant then convergence takes place at an exponential speed: this is precisely the *discrete Fourier transform.* If we desire to compute a whole range of Fourier frequencies then, indeed, FFT techniques are optimal. Having said this, the focus for our concern is altogether different, the computation of a single Fourier frequency, say, using modest number of function evaluations.

Chastened by the failure of (1.2), we might jump to the opposite conclusion and deduce that the quadrature of (1.1) for large $h\omega$ is either impossible or prohibitively expensive. The only way forward, according to this (widely shared) reasoning is to render the underlying problem into a non-oscillatory one, by dividing the interval $[0, h]$ into sufficiently large number of small subintervals (so-called “panels”) where Gauss–Christoffel quadrature can be applied with impunity. This is absolutely the wrong impression, as confirmed by Fig. 2. It displays the absolute error (in the top graph) in the integration of (1.1), again for $f(x) = \mathrm{e}^x$, with the *Filon–Legendre method* with just three integration points. (Much more about Filon-type methods in Section 3, where they will be formally defined and analysed at some length.) The situation is truly remarkable: the error is small *and it becomes smaller as the characteristic frequency grows!* The bottom figure calibrates the last statement, demonstrating that the error decays like $\mathcal{O}(\omega^{-1})$, the exact speed of decay of $I_h[\mathrm{e}^x]$.

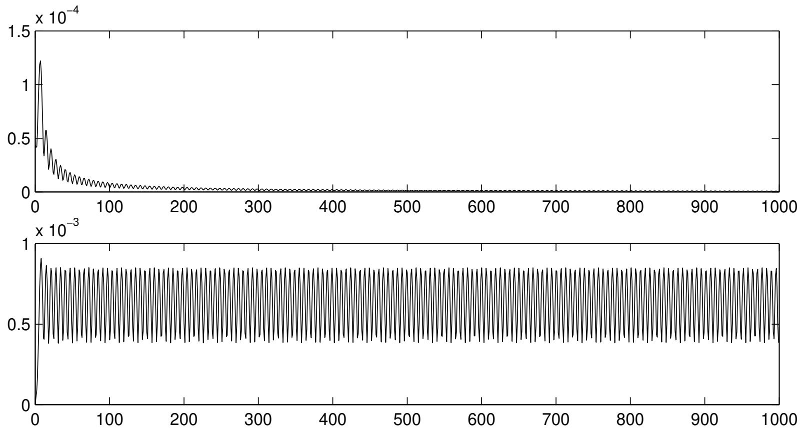

Figure 2: The error in Filon–Legendre integration of (1.1) for $f(x) = \mathrm{e}^x$, $h = \frac{1}{10}$, $\nu = 3$ and different values of ω. The top graph displays the absolute error $E_h^{\mathrm{FL}}[\mathrm{e}^x]$, the bottom the normalised error $h\omega E_h^{\mathrm{FL}}[\mathrm{e}^x]$.

This might appear remarkable and counterintuitive, but our "computational surprise" is not yet over. In Fig. 3 we have displayed the absolute error (in the top graph) for another quadrature scheme, the *Filon–Lobatto method,* again using just three function evaluations. The error decays even faster as $h\omega$ grows and the method literally revels in oscillation. Again, the bottom figure is more instructive, demonstrating that the error envelope decays proportionally to ω^{-2} when $\omega \gg 1$.

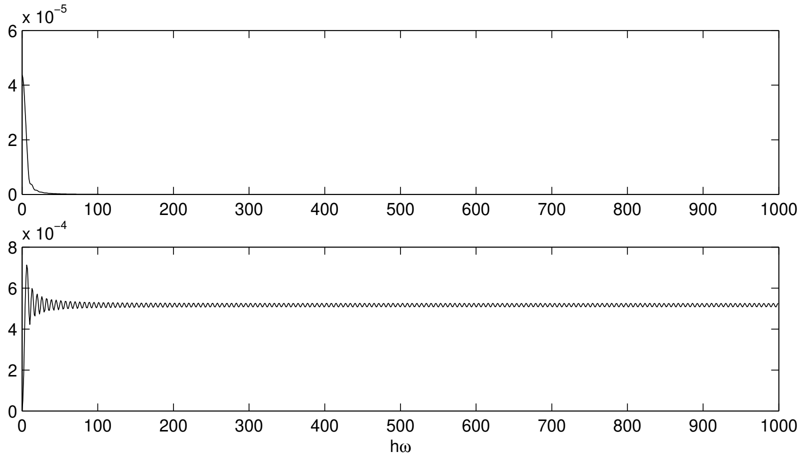

Figure 3: The error in Filon–Lobatto integration of (1.1) for $f(x) = \mathrm{e}^x$, $h = \frac{1}{10}$, $\nu = 3$ and different values of ω. The top graph displays the absolute error $E_h^{\mathrm{FL}}[\mathrm{e}^x]$, the bottom the normalised error $(h\omega)^2 E_h^{\mathrm{FL}}[\mathrm{e}^x]$.

The behaviour of Filon-type methods, as demonstrated in Figs 1–2, is not a quirk: it is, as we contend in Section 3, typical. Indeed, there are other methods, which we review in Section 4, that share this advantageous behaviour for $h\omega \gg 1$. *As long as right methods are used, quadrature of highly-oscillatory integrals is very accurate and affordable!* This is, unfortunately, not the common wisdom and we cannot resist but quote "This approach has previously been used by FILON [1], LUKE [2], and FLINN [3]. However, in the applications of the formulas developed [1, 3, 4] only those values of the mesh interval h have been used which obey the relation $|\omega|h \leq \pi/2$. Some reasons for this restriction have become apparent in the course of the work described in the present paper. These reasons may be summarized by saying that results obtained from the formulas for $|\omega|h > \pi/2$ may contain large errors, as large as the integral sought." (Clendenin 1966). This refers to specific Filon methods and the motivation for this misleading (yet unexceptional throughout the literature) statement is a Taylor expansion in powers of h for large $h\omega$, a procedure that makes no mathematical sense, followed by an examination of the leading "error" term, which has no bearing whatsoever on the actual size of the error.

Although this paper is concerned in the main with the analysis of existing methods for the quadrature of (1.1), it is valuable and instructive to commence from an application that has led the author to consider this issue at the first place, the solution of highly-oscillatory ordinary differential equations by Lie-group methods (Iserles 2002*a*, Iserles 2002*b*). Practical implementation of such methods requires in every step simultaneous quadrature of integrals of the form

$$\int_0^h f(x)\,\mathrm{d}x, \qquad \int_0^h f(x)\cos\omega x\,\mathrm{d}x, \qquad \int_0^h f(x)\sin\omega x\,\mathrm{d}x$$

for the same function f, a task for which, as will transpire in the sequel, Filon-type methods are ideally suited. Thus, we devote Section 2 to a brief description of the *modified Magnus method* from (Iserles 2002*a*), weigh its advantages and explain why the latter are bound to be lost unless the method is supplemented by a suitable quadrature technique for highly-oscillatory integrals. Both this section and Section 5 can be omitted by readers whose sole interest is in integration of (1.1), yet they provide a useful and illustrative application, inclusive of examples of specific quadrature methods, as well as being of an independent interest to readers keen to infer from quadrature of highly-oscillatory integrals to discretization of highly-oscillatory differential equations. Moreover, the computation of highly-oscillatory differential equations and highly-oscillatory integrals shares an important structural common denominator: for high frequencies, a naive Taylor expansion, implicit in the concept of 'order', provides a misleading picture of the behaviour of the error. A considerably more effective course of action is an asymptotic expansion in inverse powers of the characteristic frequency.

Section 3 is devoted to Filon-type methods. We commence from their definition: rather than describing the original special framework from (Filon 1928), we focus on the more modern and general approach of (Luke 1954) (cf. also (Bakhvalov & Vasilčeva 1968)). This is followed by detailed analysis of three situations, the *non-oscillatory regime,* where $0 < h\omega \ll 1$, the *mildly-oscillatory regime* $h\omega = \mathcal{O}(1)$ and, finally, the most interesting (from our perspective) regime, the *highly-oscillatory* one, where $h\omega \gg 1$. Our main results are as follows. Suppose that $c_1 < c_2 < \cdots < c_\nu$ are nodes in $[0,1]$ which correspond to Gauss–Christoffel quadrature of order $p \in \{\nu, \nu+1, \ldots, 2\nu\}$. Then

1. If $h\omega \gg 1$ then the quadrature error of the Filon-type method is $\mathcal{O}\big(h^{p+1}\big)$;
2. If $h\omega = \mathcal{O}(1)$ then its error is $\mathcal{O}\big(h^{\nu+1}\big)$;
3. In the case $h\omega \gg 1$ the error is $\mathcal{O}\big(h^{\nu+1}/(h\omega)\big)$, except that, once we set $c_1 = 0$ and $c_\nu = 1$, the error becomes $\mathcal{O}\big(h^{\nu+1}/(h\omega)^2\big)$.

All this is true for (1.1) and smooth functions f. As a matter of fact, we consider in Section 3 a more general integral,

$$\int_0^1 f(x)\mathrm{e}^{\mathrm{i}\omega x} w(x)\,\mathrm{d}x,$$

and our results therein depend also on the values of the nonnegative weight function w at the endpoints.

The above results fly in the face of a widespread and pernicious numerical "folk wisdom", namely that one should integrate with a fixed, moderately large number of points per period: typically, 5–7 points. This suggestion, consistent with our quote from (Clendenin 1966) (but, in fairness, we could have quoted many other references to similar effect), automatically places us in the mildly-oscillatory regime $h\omega = \mathcal{O}(1)$ which, actually, is the *worst* choice for a Filon-type method.

Filon's quadrature is not the only effective method for highly-oscillatory integrals and in Section 4 we address ourselves to two other methods. The first, due to Zamfirescu (Zamfirescu 1963, Gautschi 1968) is based on the well-known fact that an arbitrary signed measure can be represented as a difference of two Borel measures, hence the real (or imaginary) part of the complex exponential in (1.1) can be written as a difference of two positive weight functions. The latter can be integrated by two 'proper' Gauss–Christoffel quadratures (Davis & Rabinowitz 1980, Engels 1980). We analyse this technique for two choices of quadrature nodes, namely Legendre and Lobatto points, only to deduce that

1. If $0 < h\omega \ll 1$ or $h\omega = \mathcal{O}(1)$ then the quadrature error is $\mathcal{O}\big(h^{2\nu+1}\big)$ for Legendre and $\mathcal{O}\big(h^{2\nu-1}\big)$ for Lobatto;

2. If $h\omega \gg 1$ then the error is $\mathcal{O}\big(h^{\nu+1}/(h\omega)\big)$ for Legendre and $\mathcal{O}\big(h^{\nu+1}/(h\omega)^2\big)$ for Lobatto.

Note that $c_1 = 0, c_\nu = 1$ for Lobatto nodes: similarity with Filon-type methods is remarkable! Also in that section we describe a technique that has been developed by David Levin in a sequence of papers (Levin 1982, Levin 1996, Levin 1997). It rests upon collocation-based solution of a non-oscillatory solution of a certain ordinary differential equation associated with the highly-oscillating kernel. It has been demonstrated by Levin that, for $h\omega \gg 1$, the quadrature error decays like $\mathcal{O}\big(h^{\nu+1}/(h\omega)^2\big)$, once $c_1 = 0$ and $c_\nu = 1$ are selected as quadrature points. This is, as far as the current author is aware, the only instance of this phenomenon being analysed (or even observed) in numerical literature. In a very specific sense, the *leitmotif* of the present paper is to follow in Levin's footsteps and show that the choice $c_1 = 0$, $c_\nu = 1$, first observed by him and best realised by selecting Lobatto points, is optimal for the quadrature of integrals of the form (1.1), regardless of the choice of a (good) method.

In the last section we return to the modified Magnus method of Section 2, focussing on two goals. Firstly, we demonstrate how Filon-type methods can be implemented to evaluate the leading integral in a practical manner. Secondly, high-order implementation of a Magnus method requires the cubature of multivariate integrals (Iserles, Munthe-Kaas, Nørsett & Zanna 2000) and this also must be done by a method that copes well with high oscillation. Although we do not develop a general theory, along the lines of Section 3, we demonstrate through specific examples that Filon-type methods can be extended to multivariate framework.

Throughout this paper we disregard methods, some of which can be very efficient indeed, that restrict the values of ω to integer multiples of $2\pi/h$ (i.e., to the 'genuine' Fourier transform) and where such restriction is vital to the success of the method. It is valuable to list in this context the inversion of the Poisson summation formula by using Möbius numbers (Goldberg & Varga 1956, Lyness 1971) and a variation upon Filon's method due to Fosdick (Fosdick 1968).

We mention in passing that the main 'ideological' conclusion of our paper, namely that, properly handled, highly-oscillatory integrals are easy and simple to approximate, should come as little surprise to a mathematical analyst, with an interest in exact integrals. High oscillation is a smoothing operator, as apparent in our context from the Riemann–Lebesgue lemma. The challenge is how to take advantage of high oscillation in a numerical setting and our claim is that the answer has been available, however vaguely and implicitly, since 1928.

This paper is restricted to the computation of the most common form of highly-oscillating integral, the Fourier-transform-like (1.1) and its generalisation (3.1). A future paper will address itself to more general oscillators.

2 Lie-group methods for highly-oscillatory ODEs

Trading off generality for comprehension, our point of departure is the scalar linear nonautonomuous differential equation

$$y'' + g(t)y = 0, \quad t \geq 0, \qquad y(0) = y_0, \quad y'(0) = y_0', \tag{2.1}$$

where $\lim_{t\to\infty} g(t) = +\infty$ (similar analysis applies to large, yet bounded g), while the derivatives of g are of moderate size. A considerably more general treatment can be found in (Iserles 2002*a*).

As is well known from WKB analysis,

$$y(t) \sim \frac{\exp\left\{\mathrm{i}\int_0^t [g(x)]^{1/2}\,\mathrm{d}x\right\}}{[g(t)]^{1/4}}, \qquad t \gg 1,$$

hence high oscillation. Most discretizations methods are known to accumulate global error considerably faster, at an unacceptable rate. Thus, to specialise further, in the case of the *Airy oscillator* $y'' + ty = 0$ the global error of any fourth-order Runge–Kutta or multistep method, applied with a constant step size $h > 0$, accumulates like $h^4 t^{13/4}\chi(t)$, where χ is a generic highly-oscillating function ranging in $[-1, 1]$: this is independent of possible 'nice' features of the method, like A-stability, algebraic stability or symplecticity (Iserles 2002*a*). The fourth-order Magnus method (Iserles et al. 2000) does much better and the global error accumulates like $h^4 t^{1/4}\chi(t)$, but even better results can be obtained by modifying the Magnus method along the lines of (Iserles 2002*a*, Iserles 2002*b*), whence the global error *decays* like $h^3 t^{-1/4}\chi(t)$ for $t \gg 1$ and fixed small $h > 0$ (behaving like $h^7 t^{1/4}\chi(t)$ for fixed t and $h \to 0$): note that, although the order nominally drops for error bounds which are uniform in $t \gg 1$, it is the oscillation itself, rather than powers of h, that drives the global error down. We will see in Sections 3–4 that an identical phenomenon occurs in the context of highly-oscillatory quadrature.

The differential equation (2.1) is converted into a system of first-order ODEs,

$$\boldsymbol{y}' = A(t)\boldsymbol{y}, \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0, \tag{2.2}$$

where

$$A(t) = \begin{bmatrix} 0 & 1 \\ -g(t) & 0 \end{bmatrix}, \qquad \boldsymbol{y}_0 = \begin{bmatrix} y_0 \\ y_0' \end{bmatrix}.$$

Suppose that we have already computed $\boldsymbol{y}_N \approx \boldsymbol{y}(t_N)$ and wish to advance the numerical solution to $t_{N+1} = t_N + h$. We commence by computing $\tilde{A} = A(t_{N+\kappa})$, where $\kappa \in [0, 1]$. ($\kappa = \frac{1}{2}$ is an excellent choice and it leads to the favourable global-error estimates above, but $\kappa = 0$ is preferable for a nonlinear version of this method.) Next, we change the frame of reference by letting

$$\boldsymbol{y}(t) = \mathrm{e}^{(t-t_N)\tilde{A}}\boldsymbol{x}(t - t_N), \qquad t_N \leq t \leq t_{N+1}.$$

We treat $\boldsymbol{x}$ as our new unknown and observe that it itself obeys another linear differential equation,

$$\boldsymbol{x}' = B(\tau)\boldsymbol{x}, \quad \tau \geq t_N, \qquad \boldsymbol{x}(t_N) = \boldsymbol{y}_N, \tag{2.3}$$

where

$$B(\tau) = \mathrm{e}^{-\tau\tilde{A}}[A(t_N+\tau) - \tilde{A}]\mathrm{e}^{\tau\tilde{A}}, \qquad \tau \geq 0.$$

This change of variables is valid for any linear system (2.2), regardless of dimensionality and the precise form of the matrix A, and can be extended to nonlinear systems as well. However, for linear systems inherited from the linear oscillator (2.1) the new vector field B can be computed explicitly,

$$B(\tau) = [g(t_{N+\kappa}) - g(t_N+\tau)] \begin{bmatrix} \frac{1}{2}\phi^{-1}\sin 2\phi\tau & \phi^{-2}\sin^2\phi\tau \\ -\cos^2\phi\tau & -\frac{1}{2}\phi^{-1}\sin 2\phi\tau \end{bmatrix}, \tag{2.4}$$

where $\phi = g(t_{N+\kappa})]^{1/2}$.

We apply a Magnus method to the modified equation (2.3). The *Magnus expansion* is

$$\Omega(\tau) = \int_0^\tau B(x)\,\mathrm{d}x - \tfrac{1}{2}\int_0^\tau\int_0^{x_1}[B(x_2), B(x_1)]\,\mathrm{d}x_2\,\mathrm{d}x_1 + \cdots, \tag{2.5}$$

where $\boldsymbol{x}(\tau) = \mathrm{e}^{\Omega(\tau)}\boldsymbol{y}_N$, $\tau \geq 0$ (Iserles et al. 2000). Thus, to approximate $\Omega(h)$, we need to truncate the expansion in (2.5) and replace integrals by quadrature. Once a suitable approximation $\hat{\Omega} \approx \Omega(h)$ is available, we let

$$\boldsymbol{y}_{N+1} = \mathrm{e}^{h\tilde{A}}\mathrm{e}^{\hat{\Omega}}\boldsymbol{y}_N.$$

The 2×2 matrix exponentials can be easily written down explicitly.

The secret of the success of 'standard' Magnus integrators is that all underlying multivariate integrals can be computed to high precision very economically, in a small number of function evaluations and reasonable volume of linear algebra (Iserles et al. 2000). However, the matrix function B in (2.4) is highly oscillatory for 'interesting' values of ϕ, precisely the situation when Gauss–Christoffel quadrature, which plays a central role in the implementation of 'standard' Magnus, is of little use. Sometimes it is possible to get away with exact integration, e.g. for the Airy oscillator, but a more general approach requires more substantive numerical remedy.

It is important to bear in mind that high oscillation in this context is not a curse: it is indeed the secret of the remarkable success of the modified Magnus method (Iserles 2002*b*). Usual numerical integrators perform so poorly for (2.1) because their local error is expressible in terms of high derivatives and elementary differentials, whose amplitude increases rapidly in the presence of high oscillation. Modified Magnus, on the other hand, is based upon the integration of a highly-oscillating vector field B and, after all, integration is the precise opposite of differentiation, a smoothing operator! Thus, the faster B oscillates, the smaller are Magnus integrals, thus the faster the convergence in (2.5), and the smaller the error. This is precisely the compelling reason why integration *must* be replaced by quadrature that 'respects' high oscillation and provides suitable precision in a small number of function evaluations per step.

Let $\omega = 2\phi$, $f(\tau) = g(t_{N+\kappa}) - g(t_N+\tau)$ and

$$W_{-1} = \begin{bmatrix} \frac{\mathrm{i}}{2\omega} & -\frac{1}{\omega^2} \\ -\frac{1}{4} & -\frac{\mathrm{i}}{2\omega} \end{bmatrix}, \quad W_0 = \begin{bmatrix} 0 & \frac{2}{\omega^2} \\ -\frac{1}{2} & 0 \end{bmatrix}, \quad W_1 = \begin{bmatrix} -\frac{\mathrm{i}}{2\omega} & -\frac{1}{\omega^2} \\ -\frac{1}{4} & \frac{\mathrm{i}}{2\omega} \end{bmatrix}.$$

Then

$$B(\tau) = f(\tau)[\mathrm{e}^{-\mathrm{i}\omega\tau} W_{-1} + W_0 + \mathrm{e}^{\mathrm{i}\omega\tau} W_1],$$

therefore

$$\int_0^h B(x)\mathrm{d}x = \int_0^h f(x)\mathrm{e}^{-\mathrm{i}\omega x}\,\mathrm{d}x W_{-1} + \int_0^h f(x)\,\mathrm{d}x W_0 + \int_0^h f(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x W_1 \qquad (2.6)$$

and the task in hand reduces to a quadrature of (1.1) with different values of ω but with the same function f. Similar approach will be extended in Section 5 to the double integral in (2.5). By this stage, it suffices to conclude that we wish to approximate the three integrals in (2.6), two with highly-oscillating integrand and one that does not oscillate at all, to sufficiently high precision, yet with a small number of evaluations of the function f. This motivates the work of the next two sections.

3 Filon-type methods

3.1 The definition

Let $w \in \mathrm{L}[0,1]$ be a nonnegative, sufficiently smooth nonzero function and $h > 0$ a constant. We wish to approximate the integral

$$I_h[f] = \int_0^h f(x)\mathrm{e}^{\mathrm{i}\omega x} w(x/h)\,\mathrm{d}x = h\int_0^1 f(hx)\mathrm{e}^{\mathrm{i}h\omega x} w(x)\,\mathrm{d}x, \qquad (3.1)$$

where $f \in \mathrm{L}[0,1]$ is itself sufficiently smooth. Note that this generalises (1.1) by allowing a weight function, something that can be done with little extra technical effort. We assume that $\omega > 0$ for ease of notation, but our results can be trivially extended to negative ω at the cost of minor notational inconvenience.

To set the scene for our analysis, we choose ν distinct nodes $c_1 < c_2 < \cdots < c_\nu$ in $[0,1]$ and, given

$$\gamma(t) = \prod_{l=1}^{\nu}(t - c_l) = \sum_{j=0}^{\nu}\gamma_j t^j,$$

we select $s \in \{0, 1, \ldots, \nu\}$ as the largest integer so that

$$\int_0^1 x^{j-1}\gamma(x)\,\mathrm{d}x = 0, \qquad j = 1, 2, \ldots, s.$$

In other words, $p = \nu + s$ is the order of the Gauss–Christoffel quadrature (1.2) at the above nodes.

There are two alternative ways of introducing Filon-type methods (Bakhvalov & Vasilčeva 1968, Flinn 1960, Luke 1954). Firstly, we may interpolate f by a polynomial of degree $\nu - 1$,

$$f(x) \approx \tilde{f}(x) = \sum_{k=1}^{\nu}\ell_k(x/h)f(c_k h),$$

where $\ell_k \in \mathbb{P}_{\nu-1}$ is the kth cardinal polynomial of Lagrangian interpolation,

$$\ell_k(c_j) = \begin{cases} 1, & j = k, \\ 0, & j \neq k, \end{cases} \qquad k, j = 1, 2, \ldots, \nu.$$

Once f is replaced by $\tilde{f}$ in (3.1), we obtain the *Filon-type quadrature*

$$Q_h^{\mathrm{F}}[f] = I_h[\tilde{f}] = h \sum_{l=1}^{\nu} b_l(\mathrm{i}h\omega) f(c_l h), \tag{3.2}$$

where

$$b_l(\mathrm{i}h\omega) = \int_0^1 \ell_l(x) \mathrm{e}^{\mathrm{i}h\omega x} w(x)\,\mathrm{d}x, \qquad l = 1, 2, \ldots, \nu.$$

By design,

$$E_h^{\mathrm{F}}[f] = Q_h^{\mathrm{F}}[f] - I_h[f] = 0, \qquad f \in \mathbb{P}_{\nu-1},$$

hence $E_h^{\mathrm{F}}[f] = \mathcal{O}\big(h^{\nu+1}\big)$ for every sufficiently-smooth function f. Alternatively, we can obtain exactly the same weights b_l by solving the Vandermonde system

$$\sum_{l=1}^{\nu} b_l(\mathrm{i}h\omega) c_l^m = \mu_m(h\omega), \qquad m = 0, 1, \ldots, \nu - 1, \tag{3.3}$$

where the μ_ms are the *moments*

$$\mu_m(\psi) = \int_0^1 x^m \mathrm{e}^{\mathrm{i}\psi x} w(x)\,\mathrm{d}x, \qquad m \in \mathbb{Z}_+.$$

We can think of (3.2) as the Gauss–Christoffel formula with respect to the *complex-valued weight function* $\mathrm{e}^{\mathrm{i}h\omega x} w(x)$, but this analogy with standard theory of quadrature will not carry us far. In particular, any attempt to increase order by choosing the nodes consistently with complex-valued 'orthogonality' is likely to lead to c_ks outside $[0, 1]$ and, indeed, to complex nodes. Fortunately, as we demonstrate in the next subsection, such a course of action is unnecessary and we can achieve higher order by other means.

3.2 The regime $0 < h\omega \ll 1$

Let us assume that ω is bounded, while $h \to 0$. In other words, the characteristic frequency of the system is small although, in principle, ω itself might be large. We let

$$\beta_{r,m} = \sum_{l=1}^{\nu} b_l^{(r)}(0) c_l^m, \qquad r, m \in \mathbb{Z}_+.$$

Proposition 1 *For every $r = 0, 1, \ldots, p-1$ it is true that*

$$\beta_{r,m} = \mu_{r+m}(0), \qquad m = 0, 1, \ldots, p - r - 1. \tag{3.4}$$

Proof We repeatedly differentiate (3.3) with respect to ω, whence

$$\sum_{l=1}^{\nu} b_l^{(r)}(\mathrm{i}h\omega)c_l^m = \int_0^1 x^{m+r}\mathrm{e}^{\mathrm{i}h\omega x}w(x)\,\mathrm{d}x, \qquad r \in \mathbb{Z}_+.$$

Setting $\omega = 0$ results in

$$\beta_{r,m} = \mu_{r+m}(0), \qquad m = 0,1,\ldots,\nu-1. \tag{3.5}$$

This implies that $b_1^{(r)}(0), b_2^{(r)}(0), \ldots, b_\nu^{(r)}(0)$ are interpolatory weights of Gauss–Christoffel quadrature with the weight function $x^r w(x)$. Because of the orthogonality conditions for the polynomial γ, we have

$$\int_0^1 x^{r+m}\gamma(x)w(x)\,\mathrm{d}x = 0, \qquad m = 0,1,\ldots,s-1-r$$

for $r = 0,1,\ldots,s-1$. Therefore, for $r = 0,1,\ldots,s$ the Gauss–Christoffel quadrature with the weight function $x^r w(x)$ at the nodes $c_1, c_2, \ldots, c_\nu$ has order $p-r$. Consequently (3.4) holds for $r = 0,1,\ldots,s-1$ and, because of (3.5), also for $r = s, s+1, \ldots, p-1$. □

Theorem 2 *Let f be an analytic function in the disc $|z| < h_0$ for some $h_0 > 0$ and let $\omega > 0$ be fixed. Then*

$$E_h^{\mathrm{F}}[f] = \mathcal{O}\left(h^{p+1}\right), \qquad 0 < h \ll 1, \tag{3.6}$$

where $E_h^{\mathrm{F}}[f]$ is the error of the Filon-type quadrature (3.2) and $p = \nu + s$ is the order of the Gauss–Christoffel quadrature at the nodes $c_1, c_2, \ldots, c_\nu$.

Proof By the above assumption, the Taylor series

$$f(z) = \sum_{m=0}^{\infty} \frac{f_m}{m!} z^m$$

converges for $|z| < h_0$. By design, we already know that $E_h^{\mathrm{F}}[x^m] = 0$ for $m = 0,1,\ldots,\nu-1$, therefore we may assume without loss of generality that $f_m = 0$, $m = 0,1,\ldots,\nu-1$. Since

$$\mu_m(h\omega) = \sum_{r=0}^{\infty} \frac{(\mathrm{i}h\omega)^r}{r!}\mu_{m+r}(0), \quad \sum_{l=1}^{\nu} b_l(\mathrm{i}h\omega)c_l^m = \sum_{r=0}^{\infty}\frac{(\mathrm{i}h\omega)^r}{r!}\beta_{r,m}, \qquad m \in \mathbb{Z}_+,$$

substitution into (3.1) and (3.2) respectively yields

$$\begin{aligned}
I_h[f] &= \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1}\mu_m(h\omega) = \sum_{m=\nu}^{\infty}\sum_{r=0}^{\infty} \frac{f_m}{m!r!} h^{m+r+1}(\mathrm{i}\omega)^r \mu_{m+r}(0) \\
&= \sum_{m=0}^{\infty}\left[\sum_{r=0}^{m-\nu} \frac{f_{m-r}(\mathrm{i}\omega)^r}{r!(m-r)!}\right]\mu_m(0)h^{m+1}, \\
Q_h^{\mathrm{F}}[f] &= \sum_{m=\nu}^{\infty}\frac{f_m}{m!}h^{m+1}\sum_{l=1}^{\nu} b_l(h\omega)c_l^m = \sum_{m=\nu}^{\infty}\sum_{r=0}^{\infty}\frac{f_m}{m!r!}h^{m+r+1}(\mathrm{i}\omega)^r\beta_{r,m} \\
&= \sum_{m=0}^{\infty}\left[\sum_{r=0}^{m-\nu}\frac{f_{m-r}(\mathrm{i}\omega)^r}{r!(m-r)!}\beta_{r,m-r}\right]h^{m+1}.
\end{aligned}$$

Because of (3.4), it is true that $\beta_{r,m-r} = \mu_m(0)$ for $m \le p-1$, therefore

$$E_h^{\mathrm{F}}[f] = \sum_{m=p}^{\infty} \frac{h^{m+1}}{m!} \sum_{r=0}^{m-\nu} \binom{m}{r} f_{m-r} (\mathrm{i}\omega)^r [\beta_{r,m-r} - \mu_m(0)]. \tag{3.7}$$

This proves (3.6). $\square$

The statement of the theorem can be easily extended to $\mathrm{C}^{p+1}[0,h]$ functions f, except that the error expansion (3.7) is no longer available.

The leading error term follows at once from the proof,

$$E_h^{\mathrm{F}}[f] = \frac{h^{p+1}}{p!} \sum_{r=\nu}^{p} \binom{p}{r} f_r (\mathrm{i}\omega)^{p-r} [\beta_{p-r,r} - \mu_p(0)] + \mathcal{O}\big(h^{p+2}\big)\,.$$

Letting $\omega = 0$ recovers the familiar principal error term of Gauss–Christoffel quadrature, but the formula is more interesting for nonzero ω, when it depends on several derivatives of f.

The main importance of Theorem 2 from the standpoint of highly-oscillatory integration is that, insofar as the order of approximation is concerned, Filon-type quadrature (3.2) is just as good as the more familiar Gauss–Christoffel quadrature even if the characteristic frequency of the integral (3.1) is small. In the next two subsections we discuss the instance of moderate and large characteristic frequency, when Gauss–Christoffel quadrature is useless, while, as we will see, Filon-type quadrature is very effective indeed.

3.3 The regime $h\omega = \mathcal{O}(1)$

Suppose that $\psi = h\omega = \mathcal{O}(1)$, a situation corresponding to the familiar folk remedy of choosing the interval of integration (or time step, or size of a panel in compound quadrature) as c/ω for some constant c. Substituting $\omega = \psi/h$ in (3.7), we obtain after some basic algebraic manipulation

$$E_h^{\mathrm{F}}[f] = \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1} \sum_{r=(p-m)_+}^{\infty} \frac{(\mathrm{i}\psi)^r}{r!} [\beta_{r,m} - \mu_{m+r}(0)] \tag{3.8}$$

and, with some more effort,

$$E_h^{\mathrm{F}}[f] = \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1} \left[\sum_{l=1}^{\nu} b_l(\mathrm{i}\psi) c_l^m - \mu_m(\psi) \right].$$

Thus,

$$E_h^{\mathrm{F}}[f] = \frac{f_\nu}{\nu!} h^{\nu+1} \sum_{r=p}^{\infty} \frac{(\mathrm{i}\psi)^r}{r!} [\beta_{r,\nu} - \mu_{r+\nu}(0)] + \mathcal{O}\big(h^{\nu+2}\big)$$

and the order of Filon-type quadrature reduces in this setting to ν. Yet, even this is much better than conventional Gauss–Christoffel quadrature!

3.4 The regime $h\omega \gg 1$

Small $h > 0$, yet large characteristic frequency $\psi = h\omega$: this is the make-or-break regime for any quadrature method proposed for highly-oscillating integrals of the form (3.1). The main idea is to keep $h > 0$ fixed (typically, sufficiently small) and consider the *asymptotic expansion* of the error in negative powers of ψ.

Our first result is a trivial outcome of integration by parts, yet perhaps the most fundamental to the work of this paper.

Proposition 3 *For every smooth function f and $\psi \gg 1$ it is true that*

$$\begin{aligned} I_h[f] \sim\; & \frac{f(h)w(1)\mathrm{e}^{\mathrm{i}\psi} - f(0)w(0)}{\mathrm{i}\psi} \\ & + \frac{[hf'(h)w(1) + f(h)w'(1)]\mathrm{e}^{\mathrm{i}\psi} - [hf'(0)w(0) + f(0)w'(0)]}{\psi^2} \\ & + \mathcal{O}\big(\psi^{-3}\big). \end{aligned} \tag{3.9}$$

We note in passing that if fw is analytic and h-periodic in a suitable Gevrey class and ψ is an integer multiple of 2π then, as is well known, $I_h[f]$ decays exponentially for $\psi \to \infty$. This is perfectly compatible with (3.9).

An immediate consequence of the proposition is an asymptotic expansion of moments,

$$\begin{aligned} \mu_0(\psi) &\sim \frac{w(1)\mathrm{e}^{\mathrm{i}\psi} - w(0)}{\mathrm{i}\psi} + \frac{w'(1)\mathrm{e}^{\mathrm{i}\psi} - w'(0)}{\psi^2} + \mathcal{O}\big(\psi^{-3}\big), \\ \mu_1(\psi) &\sim \frac{w(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \frac{[hw(1) + w'(1)]\mathrm{e}^{\mathrm{i}\psi} - hw(0)}{\psi^2} + \mathcal{O}\big(\psi^{-3}\big) \\ \mu_m(\psi) &\sim \frac{w(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \frac{[mhw(1) + w'(1)]\mathrm{e}^{\mathrm{i}\psi}}{\psi^2} + \mathcal{O}\big(\psi^{-3}\big), \qquad m \ge 2. \end{aligned} \tag{3.10}$$

Note that (3.10) can be alternatively derived from the asymptotic expansion of $\mu_0(\psi)$, using the differential recurrence $\mu_{m+1}(\psi) = -\mathrm{i}\mu_m'(\psi)$, $m \in \mathbb{Z}_+$.

We set

$$\rho_m(\psi) = \sum_{l=1}^{\nu} b_l(\mathrm{i}\psi)c_l^m - \mu_m(\psi), \qquad m \in \mathbb{Z}_+.$$

Therefore $\rho_m \equiv 0$ for $m = 0, 1, \ldots, \nu - 1$ and, assuming again that f is analytic, it is easy to deduce from (3.8) that

$$E_h^{\mathrm{F}}[f] = \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1} \rho_m(\psi).$$

Recall the collocation polynomial $\gamma(t) = \sum_{k=0}^{\nu} \gamma_k t^k$, $\gamma(c_l) = 0$ for $l = 1, 2, \ldots, \nu$. Since

$$\sum_{l=1}^{\nu} b_l(\mathrm{i}\psi)c_l^m \gamma(c_l) \equiv 0 \qquad \Rightarrow \qquad \sum_{k=0}^{\nu} \gamma_k \sum_{l=1}^{\nu} b_l(\mathrm{i}\psi)c_l^{m+k} \equiv 0$$

for every $m \in \mathbb{Z}_+$, it is true that

$$\sum_{k=0}^{\nu} \gamma_k \rho_{k+m}(\psi) = -\sum_{k=0}^{\nu} \gamma_k \mu_{k+m}(\psi), \qquad m \in \mathbb{Z}_+. \tag{3.11}$$

Substituting (3.10) yields

$$\sum_{k=0}^{\nu} \gamma_k \mu_k(\psi) \sim \frac{w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi} - w(0)\gamma(0)}{\mathrm{i}\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr)\,,$$

$$\sum_{k=0}^{\nu} \gamma_k \mu_{k+m}(\psi) \sim \frac{w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr)\,, \qquad m \geq 1.$$

For $m = 0$, $\rho_k \equiv 0$ for all $k \leq \nu - 1$. This, in tandem with $\gamma_\nu = 1$, implies that

$$\rho_\nu(\psi) \sim \frac{w(0)\gamma(0) - w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr)\,.$$

Proposition 4 *There exist numbers* $\{p_m\}_{m\in\mathbb{Z}_+}$ *and* $\{q_m\}_{m\in\mathbb{Z}_+}$, *not all zero, such that*

$$\rho_m(\psi) \sim \frac{p_m w(0)\gamma(0) - q_m w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr)\,, \qquad m \in \mathbb{Z}_+. \tag{3.12}$$

Proof Clearly, $p_m = q_m = 0$ for $m \leq \nu - 1$ and $p_\nu = q_\nu = 1$. (Thus, in particular, these numbers cannot all be zero.) For $m \geq 1$, (3.11) becomes

$$\sum_{k=0}^{\nu} \gamma_k \rho_{k+m}(\psi) \sim -\frac{w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr)\,.$$

Up to $\mathcal{O}\bigl(\psi^{-2}\bigr)$, this is a linear difference equation with a forcing term. Substituting (3.12) we conclude that, as long as $w(0)\gamma(0), w(1)\gamma(1) \neq 0$, it is true that

$$\sum_{k=0}^{\nu} \gamma_k p_{k+m} = 0, \qquad \sum_{k=0}^{\nu} \gamma_k q_{k+m} = -1, \qquad m \geq 1.$$

The general solution of these recurrences is

$$p_m = \sum_{k=1}^{\nu} \tilde{p}_k c_k^m, \qquad q_m = \sum_{k=1}^{\nu} \tilde{q}_k c_k^m - \frac{1}{\gamma(1)}, \qquad m \geq 0,$$

where the constants $\{\tilde{p}_k\}_{k=1}^{\nu}$ and $\{\tilde{q}_k\}_{k=1}^{\nu}$ can be determined from initial values by solving a (nonsingular) Vandermonde linear algebraic system.

If $w(0)\gamma(0) = 0$, the first equation need be replaced by $p_m \equiv 0$, while if $w(1)\gamma(1) = 0$ then, in place of the second equation, we have $q_m \equiv 0$. (This is consistent with both being zero, since then trivially $\rho_m(\psi) \sim \mathcal{O}\bigl(\psi^{-2}\bigr)$.)

We conclude that the constants stipulated in the statement of the proposition do exist and the estimate (3.12) is valid. □

We deduce from (3.12) that

$$\begin{aligned} E_h^{\mathrm{F}}[f] &= \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1} \rho_m(\psi) \\ &\sim \sum_{m=\nu}^{\infty} \frac{f_m}{m!} h^{m+1} \frac{p_m w(0)\gamma(0) - q_m w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} + \mathcal{O}\bigl(h^{\nu+1}\psi^{-2}\bigr) \\ &= \frac{w(0)\gamma(0)}{\mathrm{i}\psi} \sum_{m=\nu}^{\infty} \frac{f_m}{m!} p_m h^{m+1} - \frac{w(1)\gamma(1)\mathrm{e}^{\mathrm{i}\psi}}{\mathrm{i}\psi} \sum_{m=\nu}^{\infty} \frac{f_m}{m!} q_m h^{m+1} + \mathcal{O}\bigl(h^{\nu+1}\psi^{-2}\bigr)\,. \end{aligned}$$

Set

$$\tilde{f}(x) = \sum_{m=\nu}^{\infty} \frac{f_m}{m!} x^m,$$

the *essential part* of the function f: note that $E_h^{\mathrm{F}}[\tilde{f}] = E_h^{\mathrm{F}}[f]$ regardless of the size of h and ω. Using the values of the p_ms and q_ms from the proof of Proposition 4, we readily have

$$\begin{aligned} E_h^{\mathrm{F}}[f] &\sim \frac{h}{\mathrm{i}\psi}\left[w(0)\gamma(0)\sum_{k=1}^{\nu}\tilde{p}_k\tilde{f}(c_k h) - w(1)\gamma(1)\sum_{m=1}^{\nu}\tilde{q}_k\tilde{f}(c_k h) + w(1)\tilde{f}(h)\right] \\ &\quad + \mathcal{O}\big(h^{\nu+1}\psi^{-2}\big) \\ &= \frac{f_\nu h^{\nu+1}}{\nu!\mathrm{i}\psi}\left[w(0)\gamma(0)\sum_{k=1}^{\nu}\tilde{p}_k c_k^\nu - w(1)\gamma(1)\sum_{k=1}^{\nu}\tilde{q}_k c_k^\nu + w(1)\right] \\ &\quad + \mathcal{O}\big(h^{\nu+2}\psi^{-1}, h^{\nu+1}\psi^{-2}\big)\,. \end{aligned} \tag{3.13}$$

This is true for $w(0)\gamma(0), w(1)\gamma(1) \neq 0$. In the remaining cases,

$$\left.\begin{array}{l} w(0)\gamma(0)=0, \\ w(1)\gamma(1)\neq 0 \end{array}\right\} \qquad E_h^{\mathrm{F}}[f] \sim \frac{w(1)h}{\mathrm{i}\psi}\left[\tilde{f}(h) - \gamma(1)\sum_{k=1}^{\nu}\tilde{q}_k\tilde{f}(c_k h)\right] + \mathcal{O}\big(h^{\nu+1}\psi^{-2}\big)\,,$$

$$\left.\begin{array}{l} w(0)\gamma(0)\neq 0, \\ w(1)\gamma(1)= 0 \end{array}\right\} \qquad E_h^{\mathrm{F}}[f] \sim \frac{w(0)\gamma(0)h}{\mathrm{i}\psi}\sum_{k=1}^{\nu}\tilde{p}_k\tilde{f}(c_k h) + \mathcal{O}\big(h^{\nu+1}\psi^{-2}\big)\,,$$

$$\left.\begin{array}{l} w(0)\gamma(0)=0, \\ w(1)\gamma(1)= 0 \end{array}\right\} \qquad E_h^{\mathrm{F}}[f] \sim \mathcal{O}\big(h^{\nu+1}\psi^{-2}\big)\,.$$

The stage is now set to formulate perhaps the most interesting result with regard to the Filon-type quadrature (3.2).

Theorem 5 *If (a) either $w(0) = 0$ or $c_1 = 0$, and (b) either $w(1) = 0$ or $c_\nu = 1$, then $E_h^{\mathrm{F}}[f] \sim \mathcal{O}\big(h^{\nu+1}\psi^{-2}\big)$, otherwise $E_h^{\mathrm{F}}[f] \sim \mathcal{O}\big(h^{\nu+1}\psi^{-1}\big)$. Moreover, unless $w(1) = 0$ and either $w'(1) = 0$ or $c_\nu = 1$, there exists no choice of quadrature nodes that gives $E_h^{\mathrm{F}}[f] \sim \mathcal{O}\big(h^{\nu+1}\psi^{-3}\big)$ for general, sufficiently-smooth function f.*

Proof Following our analysis, it remains just to prove the impossibility of error decay being faster than $\mathcal{O}\big(\psi^{-2}\big)$. To this end we use (3.10) to calculate the ψ^{-2} term in $\sum_{k=0}^{\nu}\gamma_k\mu_{k+m}(\psi)$ for $m \geq 2$, namely

$$\frac{[mhw(1) + w'(1)]\gamma(1) + hw(1)\gamma'(1)}{\psi^2}\mathrm{e}^{\mathrm{i}\psi}.$$

Progressing like in our treatment of the ψ^{-1} term, we need to choose quadrature nodes to annihilate the above expression. Since all quadrature nodes are simple and in $[0, 1]$, it is obvious that $\gamma'(1) \neq 0$ and this expression cannot be annihilated unless the conditions $w(1) = 0$ and either $w'(1) = 0$ or $c_\nu = 1$ hold. □

Assembling the results of this section together, we have determined the rate of decay of quadrature error in the three regimes of characteristic frequency,

1. If $0 < h\omega \ll 1$ then $E_h^{\mathrm{F}}[f] = \mathcal{O}\big(h^{p+1}\big)$, where p is the order of the underlying Gauss–Christoffel quadrature;

2. If $h\omega = \mathcal{O}(1)$ then $E_h^{\mathrm{F}}[f] = \mathcal{O}\big(h^{\nu+1}\big)$;

3. If $h\omega \gg 1$ then $E_h^{\mathrm{F}}[f] = \mathcal{O}\big(h^{\nu+1}/\psi\big)$, unless both $c_1 w(0) = 0$ and $(1 - c_\nu)w(1) = 0$, in which case $E_h^{\mathrm{F}}[f] = \mathcal{O}\big(h^{\nu+1}/\psi^2\big)$.

Consequently, for general weight functions, the optimal choice, maximising error decay throughout the three regimes, is that of *Lobatto* points: $c_1 = 0$, $c_\nu = 1$ and $c_2, \ldots, c_{\nu-1}$ chosen so that the overall order of quadrature is $2\nu - 2$ (Davis & Rabinowitz 1980). If the weight function vanishes at one endpoint, we can increase the order in the non-oscillatory regime by one, choosing *Radau points.* If $w(0) = w(1) = 0$, though, it is best to use *Gauss points,* thereby attaining order 2ν in the non-oscillatory regime.

4 Other methods for highly-oscillatory integrals

Many methods have been proposed for the quadrature of highly-oscillatory integrals. We intend to disregard all methods that reduce the problem in hand to a (large) number of non-oscillatory integrals, since the analysis of the last section strongly implies that this is far from optimal. Moreover, we consider neither methods that employ higher derivatives of f, although such methods can be exceedingly effective when higher derivatives are easily available (Davis & Rabinowitz 1980), nor methods that are valid only when $h\omega$ is an integer multiple of 2π, an issue upon which we have remarked in Section 1. It is not the purpose of this section to provide a brief survey of methods for highly-oscillatory integrals, but to focus on two alternative approaches which, remarkably, share the behaviour of Filon-type methods for large characteristic frequencies.

4.1 Zamfirescu's method

Let us focus for simplicity's sake on the real oscillator

$$I_h[f] = h \int_0^1 f(hx) \sin \omega h x \, \mathrm{d}x. \tag{4.1}$$

Following (Zamfirescu 1963) (cf. also (Davis & Rabinowitz 1980, Engels 1980, Gautschi 1968)), we write it in the form $I_h[f] = I_h^{(2)}[f] - I_h^{(1)}[f]$, where

$$I_h^{(1)}[f] = h \int_0^1 f(hx)\, \mathrm{d}x, \quad I_h^{(2)}[f] = h \int_0^1 f(x)(1 + \sin \omega h x)\, \mathrm{d}x.$$

All this is nothing but the well-known representation of an arbitrary function, in our instance $\sin \omega h x$, as a difference of two positive functions, and can be transparently extended to other highly-oscillatory integrals.

The weight functions in both $I_h^{(1)}$ and $I_h^{(2)}$ are positive, hence we may approximate the two integrals with Gauss–Christoffel quadrature (1.2). In other words, we let $c_1^{(j)}, c_2^{(j)}, \ldots, c_\nu^{(j)}$

and $b_1^{(j)}, b_2^{(j)}, \ldots, b_\nu^{(j)}$ be the nodes and the weights of a Gauss–Christoffel quadrature for $I_h^{(j)}$, $j = 1, 2$, whence

$$Q_h^z[f] = h \sum_{l=1}^{\nu} b_l^{(2)} f(c_l^{(2)} h) - h \sum_{l=1}^{\nu} b_l^{(1)} f(c_l^{(1)} h). \tag{4.2}$$

Note that the $c_l^{(2)}$s and $b_l^{(2)}$s both depend upon $h\omega$. For simplicity we assume that the $c_l^{(1)}$s and $b_l^{(1)}$s are independent of ψ. It makes sense to require that the two quadratures are *compatible:* $c_l^{(2)}(0) = c_l^{(1)}$, $l = 1, 2, \ldots, \nu$.

We let $\gamma^{(j)}(t) = \prod_{k=1}^{\nu}(t - c_k^{(j)})$, $j = 1, 2$, and assume that each Gauss–Christoffel quadrature in (4.2) is of order $p = \nu + s$. This requires

$$\int_0^1 x^m \gamma^{(1)}(x)\,\mathrm{d}x = \int_0^1 x^m \gamma^{(2)}(x; h\omega) \sin \omega h x\,\mathrm{d}x = 0, \qquad m = 0, 1, \ldots, s-1.$$

As before, we write $\psi = h\omega$ wherever this is convenient.

It is a straightforward consequence of our construction that the error is $\mathcal{O}\big(h^{p+1}\big)$ when *either* ω or $h\omega$ are fixed, while $h \to 0$. Yet, more interesting from our point of view is the highly-oscillatory regime $\psi = h\omega \gg 1$.

Rather than taking the most general route, we herewith restrict our attention to just two kinds of quadrature, the *Gauss–Legendre* scheme, whereby $s = \nu$, and the *Lobatto* method, with $c_1 = 0$, $c_\nu = 1$ and $s = \nu - 2$. The purpose of this paper is to understand Filon-type quadrature from Section 3, the present method is included here mainly for comparison, and there is little justification in embarking presently on a more comprehensive analysis.

We commence from the *Gauss–Legendre* quadrature, whence $\gamma^{(1)}$ is a scalar multiple of P_ν, the Legendre polynomial shifted to the interval $[0,1]$. The order conditions for $\gamma^{(2)}$ read

$$\int_0^1 x^m \gamma^{(2)}(x)\,\mathrm{d}x + \int_0^1 x^m \gamma^{(2)}(x) \sin \psi x\,\mathrm{d}x = 0, \qquad m = 0, 1, \ldots, \nu - 1,$$

where, as before, $\psi = h\omega$. Integrating by parts, we easily confirm that

$$\int_0^1 x^m \gamma^{(2)}(x) \sin \psi x\,\mathrm{d}x \sim \frac{\gamma^{(2)}(1)\cos\psi - 0^m \gamma^{(2)}(0)}{\psi} + \mathcal{O}\big(\psi^{-2}\big)\,.$$

Note that $\gamma^{(2)}(0), \gamma^{(2)}(1) \neq 0$, since zeros of orthogonal polynomials reside in the *open* support of the weight function. Therefore

$$\int_0^1 x^m \gamma^{(2)}(x)\,\mathrm{d}x \sim \mathcal{O}\big(\psi^{-1}\big)\,, \qquad m = 0, 1, \ldots, \nu - 1,$$

and we deduce from the implicit function theorem that there exist $\delta_1, \delta_2, \ldots, \delta_\nu \in \mathrm{L}[0, \infty)$, not all zero, such that

$$c_l^{(2)} \sim c_l^{(1)} + \frac{\delta_l(\psi)}{\psi} + \mathcal{O}\big(\psi^{-2}\big)\,, \qquad l = 1, 2, \ldots, \nu.$$

Moreover, since the weights are formed by solving a Vandermonde linear system, there also exist $\beta_1, \beta_2, \ldots, \beta_\nu \in \mathrm{L}[0,\infty)$ such that

$$b_l^{(2)} \sim b_l^{(1)} + \frac{\beta_l(\psi)}{\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr), \qquad l = 1, 2, \ldots, \nu.$$

Therefore

$$\begin{aligned} Q_h^{\mathrm{z}}[f] &= h\sum_{l=1}^{\nu} b_l^{(2)} f(c_l^{(2)}h) - h\sum_{l=1}^{\nu} b_l^{(1)} f(c_l^{(1)}h) \\ &\sim h\sum_{l=1}^{\nu}[b_l^{(1)} + \psi^{-1}\beta_l] f(c_l^{(1)}h + h\psi^{-1}\delta_l) - h\sum_{l=1}^{\nu} b_l^{(1)} f(c_l^{(1)}h) + \mathcal{O}\bigl(\psi^{-2}\bigr) \\ &= \frac{h}{\psi}\sum_{l=1}^{\nu}[\beta_l(\psi) f(c_l^{(1)}h) + h b_l^{(1)}\delta_l(\psi) f'(c_l^{(1)}h)] + \mathcal{O}\bigl(\psi^{-2}\bigr). \end{aligned}$$

On the other hand, integrating by parts,

$$I_h[f] \sim h\frac{f(h)\cos\psi - f(0)}{\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr), \qquad \psi \gg 1, \tag{4.3}$$

Hence the $\mathcal{O}\bigl(\psi^{-1}\bigr)$ term cannot be annihilated for all f, regardless of the choice of the ψ-dependent coefficients, and we deduce that the quadrature error decays like $\mathcal{O}\bigl(\psi^{-1}\bigr)$.

The situation is somewhat different for Lobatto quadrature. We revisit our analysis of Gauss–Legendre, replacing $s = \nu$ with $s = \nu - 2$ throughout. Since now $\gamma^{(2)}(0) = \gamma^{(1)}(2) = 0$, we have $\int_0^1 x^m \gamma^{(2)}(x)\,\mathrm{d}x \sim \mathcal{O}\bigl(\psi^{-2}\bigr)$, therefore

$$c_l^{(2)} \sim c_l^{(1)} + \mathcal{O}\bigl(\psi^{-2}\bigr), \qquad l = 1, 2, \ldots, \nu.$$

Letting, as before, $b_l^{(2)} \sim b_l^{(1)} + \psi^{-1}\beta_l + \mathcal{O}\bigl(\psi^{-2}\bigr)$, interpolatory conditions for the weights thus imply that

$$\begin{aligned} \sum_{l=1}^{\nu}[b_l^{(1)} + \psi^{-1}\beta_l] c_l^{(1)^m} &\sim \int_0^1 x^m(1 + \sin\psi x)\,\mathrm{d}x + \mathcal{O}\bigl(\psi^{-2}\bigr) \\ &\sim \frac{1}{m+1} + \frac{\cos\psi - 0^m}{\psi} + \mathcal{O}\bigl(\psi^{-2}\bigr). \end{aligned}$$

Therefore, up to $\mathcal{O}\bigl(\psi^{-1}\bigr)$,

$$\sum_{l=1}^{\nu} \beta_l c_l^{(1)^m} \sim \begin{cases} \cos\psi - 1, & m = 0, \\ \cos\psi, & m = 1, 2, \ldots, \nu - 1. \end{cases}$$

Subtracting the equation for m from that for $m-1$ for $m = 2, 3, \ldots, \nu - 1$, we have

$$\sum_{l=1}^{\nu} c_l^{(1)}[1 - c_l^{(1)}]\beta_l c_l^{(1)^m} \sim \mathcal{O}\bigl(\psi^{-1}\bigr), \qquad m = 0, 1, \ldots, \nu - 3.$$

Recall, however, that $c_l^{(1)} = 0$, $c_\nu^{(1)} = 1$. Therefore we have $\nu - 2$ 'asymptotic equations' in the variables $\beta_2, \beta_3, \ldots, \beta_{\nu-1}$ with a nonsingular Vandermonde matrix and deduce that

$$\beta_l(\psi) \sim \mathcal{O}\big(\psi^{-1}\big), \qquad l = 2, 3, \ldots, \nu - 1.$$

In other words, β_ls for this range of l do not feature in the $\mathcal{O}\big(\psi^{-1}\big)$ expansion term: just β_1 and β_ν are left. Substituting $c_l^{(1)} = 0$, $c_\nu^{(1)} = 1$ into the equations for $m = 0, 1$ we obtain

$$\beta_1(\psi) \sim -1 + \mathcal{O}\big(\psi^{-1}\big), \qquad \beta_\nu(\psi) \sim \cos\psi + \mathcal{O}\big(\psi^{-1}\big).$$

This results in

$$\begin{aligned}
Q_h^{\mathrm{z}}[f] &= h \sum_{l=1}^{\nu} b_l^{(2)} f(c_l^{(2)} h) - h \sum_{l=1}^{\nu} b_l^{(1)} f(c_l^{(1)} h) \\
&\sim h \left\{ \left[b_l^{(1)} - \frac{1}{\psi} \right] f(0) + \sum_{l=2}^{\nu-1} b_l^{(1)} f(c_l^{(1)} h) + \left[b_\nu^{(1)} + \frac{\cos\psi}{\psi} \right] f(h) \right\} \\
&\quad - h \sum_{l=1}^{\nu} b_l^{(1)} f(c_l^{(1)} h) + \mathcal{O}\big(\psi^{-2}\big) \\
&= h \frac{f(h)\cos\psi - f(0)}{\psi} + \mathcal{O}\big(\psi^{-2}\big).
\end{aligned}$$

Comparison with (4.3) confirms that the error decays like $\mathcal{O}\big(\psi^{-2}\big)$.

Note that we have neither computed explicitly an integer $r \geq 1$, say, such that the error decay is $\mathcal{O}\big(h^r \psi^{-1}\big)$ or $\mathcal{O}\big(h^r \psi^{-2}\big)$ for Gauss–Legendre and Lobatto, respectively, nor considered higher-order terms in the asymptotic expansion. The work of this subsection lays no claims to have treated the method (4.2) as comprehensively as our analysis of Filon-type methods in Section 3. Insofar as this paper is concerned, our main conclusion is that the choice $c_1 = 0$, $c_\nu = 1$, leads to the most rapid attenuation of the error for large characteristic frequency, behaviour which is identical to that of Filon-type methods and which we will encounter again in the next subsection.

We conclude this brief analysis of (4.2) with two remarks. Firstly, have we taken

$$I_h[f] = h \int_0^1 f(hx) \cos\omega h x \, \mathrm{d}x$$

in place of (4.1), the $\mathcal{O}\big(\psi^{-2}\big)$ error decay could have been obtained with a Radau scheme (thus, fixing $c_\nu^{(1)} = c_\nu^{(2)} = 1$ and requiring order $2\nu - 1$) in place of Lobatto. Secondly, on the face of it, (4.2) is better than the Filon-type method (3.2), at least in the mildly-oscillatory regime $h\omega = \mathcal{O}(1)$. This is misleading since the method of Zamfirescu requires roughly twice the number of function evaluations for (4.1) and roughly trice for the complex integral (3.1).

4.2 Levin's method

In a series of papers that should have elicited more attention, David Levin addressed himself to the quadrature of highly-oscillatory integrals, introducing a new collocation-based algorithm and observing that once $c_1 = 0$ and $c_\nu = 1$ are collocation points, the error decays like $\mathcal{O}(\psi^{-2})$ (Levin 1982, Levin, Reichel & Ringhoffer 1984, Levin 1996, Levin 1997). (Cf. (Evans & Chung 2003) for a recent generalisation.) Note that, although the method "follows the spirit of Filon's method" (Levin 1982), it is genuinely different from the latter.

Although Levin's method can be generalised a great deal, we restrict ourselves to the framework of the present paper and briefly describe the 'plain vanilla' method for the integral (3.1) with the trivial weight function $w \equiv 1$. Suppose that we know the solution of the ordinary differential system

$$y' + \mathrm{e}^{\mathrm{i}h\omega x} y = f, \tag{4.4}$$

with an arbitrary initial condition. Then

$$I_h[f] = h[y(1)\mathrm{e}^{\mathrm{i}h\omega} - y(0)].$$

In other words, solving (4.4) is equivalent to integrating (3.1). Levin proposes to approximate

$$y(x) \approx \tilde{y}(x) = \sum_{k=1}^{\nu} y_k \varphi_k(x),$$

where $\{\varphi_1, \varphi_2, \ldots, \varphi_\nu\}$ are suitable linearly-independent functions, and impose the differential equation solely at the ν *collocation points* $c_1 < c_2 < \cdots < c_\nu$,

$$\tilde{y}'(c_m) + \mathrm{i}h\omega\tilde{y}(c_m) = f(hc_m), \qquad m = 1, 2, \ldots, \nu.$$

This reduces to the linear algebraic system

$$\sum_{k=1}^{\nu} [\varphi_k'(c_m) + \mathrm{i}h\omega\varphi_k(c_m)] y_k = f(c_m h), \qquad m = 1, 2, \ldots, \nu$$

which, once it has been solved, leads to the quadrature

$$Q_h^{\mathrm{L}}[f] = h[\tilde{y}(1)\mathrm{e}^{\mathrm{i}h\omega} - \tilde{y}(0)]. \tag{4.5}$$

Levin proves that setting $c_1 = 0$ and $c_\nu = 1$ results in error attenuation of $\mathcal{O}(\psi^{-2})$ for $\psi = h\omega \gg 1$.

Although we can write $Q_h^{\mathrm{L}}[f]$ as a linear combination of function values with $(h\omega)$-dependent weights, it is in general different from a Filon-type quadrature even if we attempt to follow the 'polynomial reasoning' of the latter by choosing $\varphi_k(x) = x^{k-1}$, $k = 1, 2, \ldots, \nu$. For Lobatto weights with $\nu = 2$ and $\nu = 3$, however, both methods coincide (for brevity we again substitute $\psi = h\omega$), with the weights

$$b_1(\psi) = \frac{\mathrm{i}}{\psi} + \frac{1 - \mathrm{e}^{\mathrm{i}\psi}}{\psi^2}, \qquad b_2(\psi) = -\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\psi}}{\psi} + \frac{1 - \mathrm{e}^{\mathrm{i}\psi}}{\psi^2}.$$

and

$$\begin{aligned}
b_1(\psi) &= \frac{\mathrm{i}}{\psi} + \frac{3 + \mathrm{e}^{\mathrm{i}\psi}}{\psi^2} - \frac{4\mathrm{i}(1 - \mathrm{e}^{\mathrm{i}\psi})}{\psi^3}, \\
b_2(\psi) &= -\frac{4(1 + \mathrm{e}^{\mathrm{i}\psi})}{\psi^2} + \frac{8\mathrm{i}(1 - \mathrm{e}^{\mathrm{i}\psi})}{\psi^3}, \\
b_3(\psi) &= -\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\psi}}{\psi} + \frac{1 + 3\mathrm{e}^{\mathrm{i}\psi}}{\psi^2} - \frac{4\mathrm{i}(1 - \mathrm{e}^{\mathrm{i}\psi})}{\psi^3}.
\end{aligned}$$

respectively. As a matter of fact, the two quadratures are identical for $\nu = 2$ for *all* weights but, lest a conjecture starts to form by this stage in a reader's mind, Gauss–Legendre nodes lead to different quadratures for $\nu = 3$.

5 Lie-group methods revisited

Our point of departure is the Magnus expansion (2.5) of the modified equation (2.3) and we consider two options. Firstly, we truncate all but the first integral. This results in a method of 'classical' order four: although there is an order reduction once we form asymptotic estimates for $\phi \gg 1$, we still need to discretise the integral consistently with the order of the method. To this end, we may use the Filon–Lobatto quadrature with $\nu = 3$ from the last section. Note that although its implementation nominally requires three function evaluations, in reality just two are needed per time step, since we can reuse a single function evaluation of g from the previous step: this phenomenon, known as 'FSAL' (First Same As Last) is familiar from the practice of Runge–Kutta methods for ordinary differential equations (Hairer, Nørsett & Wanner 1993). Moreover, letting $\kappa = \frac{1}{2}$ means that the mid-point calculation of g can be used both for modification of the original equation and for quadrature: actually, in that case $f(\frac{1}{2}h) = 0$. Recall further from (2.6) that we need to compute three integrals: with little additional algebra we obtain

$$\int_0^h B(x)\,\mathrm{d}x = -\int_0^h f(x)\cos\omega x\,\mathrm{d}x \begin{bmatrix} 0 & \frac{2}{\omega^2} \\ \frac{1}{2} & 0 \end{bmatrix} + \int_0^h f(x)\,\mathrm{d}x \begin{bmatrix} 0 & \frac{2}{\omega^2} \\ -\frac{1}{2} & 0 \end{bmatrix}$$
$$+ \int_0^h f(x)\sin\omega x\,\mathrm{d}x \begin{bmatrix} \frac{1}{\omega} & 0 \\ 0 & -\frac{1}{\omega} \end{bmatrix}.$$

Letting

$$\begin{aligned} b_1^{(1)} &= \frac{3+\cos\psi}{\psi^2} - \frac{4\sin\psi}{\psi^3}, & b_1^{(2)} &= \frac{1}{\psi} + \frac{\sin\psi}{\psi^2} - \frac{4(1-cos\psi)}{\psi^3} \\ b_2^{(1)} &= -\frac{4(1+\cos\psi)}{\psi^2} + \frac{8\sin\psi}{\psi^3}, & b_2^{(2)} &= -\frac{4\sin\psi}{\psi^2} + \frac{8(1-\cos\psi)}{\psi^3} \\ b_3^{(1)} &= \frac{\sin\psi}{\psi} + \frac{1+3\cos\psi}{\psi^2} - \frac{4\sin\psi}{\psi^3}, & b_3^{(2)} &= -\frac{\cos\psi}{\psi} + \frac{3\sin\psi}{\psi^2} - \frac{4(1-\cos\psi)}{\psi^3}, \end{aligned}$$

where $\psi = h\omega$, we have

$$\int_0^h f(x)\cos\omega\,\mathrm{d}x \approx h[b_1^{(1)}f(0) + b_2^{(1)}f(\tfrac{1}{2}h) + b_3^{(1)}f(h)],$$
$$\int_0^h f(x)\sin\omega\,\mathrm{d}x \approx h[b_1^{(2)}f(0) + b_2^{(2)}f(\tfrac{1}{2}h) + b_3^{(2)}f(h)],$$
$$\int_0^h f(x)\,\mathrm{d}x \approx h[\tfrac{1}{6}f(0) + \tfrac{2}{3}f(\tfrac{1}{2}h) + \tfrac{1}{6}f(h)],$$

all fourth-order quadratures.

A possible alternative to the above is to exploit the fact that f vanishes at $\frac{1}{2}h$. Letting $\bar{f}(x) = f(x)/(x - \frac{1}{2}h)$, we need to evaluate

$$h\int_0^h \bar{f}(x)\left\{\begin{array}{c}1\\ \cos\omega x\\ \sin\omega x\end{array}\right\} w(x/h)\,\mathrm{d}x = h^2\int_0^1 \bar{f}(hx)\left\{\begin{array}{c}1\\ \cos\omega hx\\ \sin\omega hx\end{array}\right\} w(x)\,\mathrm{d}x,$$

where $w(x) = x - \frac{1}{2}$, a *signed* weight function. In general, the analysis of Section 3 is not valid for signed weights, since the classical theory of Gauss–Christoffel quadrature loses its validity within this setting (Gautschi 1981). In our particular case, however, it is possible to derive a fourth-order Lobatto method of this kind with just two quadrature points, $c_1 = 0$ and $c_2 = 1$. Upon close examination, however, this turns out to be precisely the Lobatto method from the previous paragraph.

A sixth-order modified Magnus scheme reads, prior to quadrature, $\boldsymbol{y}_{N+1} = \mathrm{e}^{h\tilde{A}}\mathrm{e}^{\Omega(h)}\boldsymbol{y}_N$, where

$$\Omega(h) = \int_0^h B(x)\,\mathrm{d}x - \tfrac{1}{2}\int_0^h\int_0^{x_1}[B(x_2), B(x_1)]\,\mathrm{d}x_2\,\mathrm{d}x_1.$$

Both above integrals need be approximated to order six. Insofar as the first integral is concerned, we use again a Lobatto scheme, this time with $\nu = 4$, namely

$$c_1 = 0, \qquad c_2 = \tfrac{1}{2} - \tfrac{\sqrt{5}}{10}, \qquad c_3 = \tfrac{1}{2} + \tfrac{\sqrt{5}}{10}, \qquad c_4 = 1.$$

In the case when $f(\frac{1}{2}h) = 0$, however, we can use at exactly the same price in function evaluations an eighth-order Lobatto scheme with $\nu = 5$ and

$$c_1 = 0, \qquad c_2 = \tfrac{1}{2} - \tfrac{\sqrt{21}}{14}, \qquad c_3 = \tfrac{1}{2}, \qquad c_4 = \tfrac{1}{2} + \tfrac{\sqrt{21}}{14}, \qquad c_5 = 1. \tag{5.1}$$

This is the course of action that we adopt in the sequel. The (straightforward) derivation of the weights is of little interest.

The calculation of the double integral is more of a challenge, yet it can be also addressed by our techniques. We commence by deducing from (2.6) that

$$\int_0^{x_1}[B(x_2), B(x_1)]\,\mathrm{d}x_2 = \zeta_{-1,0}(x_1)[W_{-1}, W_0] + \zeta_{-1,1}(x_1)[W_{-1}, W_1] + \zeta_{0,1}(x_1)[W_0, W_1],$$

where

$$\begin{aligned}
\zeta_{-1,0}(x) &= \int_0^x f(x)f(y)[\mathrm{e}^{-\mathrm{i}\omega y} - \mathrm{e}^{-\mathrm{i}\omega x}]\,\mathrm{d}y,\\
\zeta_{-1,1}(x) &= \int_0^x f(x)f(y)[\mathrm{e}^{\mathrm{i}\omega(x-y)} - \mathrm{e}^{\mathrm{i}\omega(y-x)}]\,\mathrm{d}y = 2\mathrm{i}\int_0^x f(x)f(y)\sin\omega(x-y)\,\mathrm{d}y,\\
\zeta_{0,1}(x) &= \int_0^x f(x)f(y)[\mathrm{e}^{\mathrm{i}\omega x} - \mathrm{e}^{\mathrm{i}\omega y}]\,\mathrm{d}y.
\end{aligned}$$

Moreover,

$$[W_{-1}, W_0] = \mathrm{i}U_1 - U_2, \qquad [W_{-1}, W_1] = -\mathrm{i}U_1, \qquad [W_0, W_1] = \mathrm{i}U_1 + U_2,$$

where

$$U_1 = \begin{bmatrix} 0 & \frac{2}{\omega^3} \\ \frac{1}{2\omega} & 0 \end{bmatrix}, \qquad U_2 = \begin{bmatrix} -\frac{1}{\omega^2} & 0 \\ 0 & \frac{1}{\omega^2} \end{bmatrix}.$$

After some algebra, everything simplifies to

$$\begin{aligned} \int_0^h \int_0^{x_1} [B(x_2), B(x_1)] \, \mathrm{d}x_2 \, \mathrm{d}x_1 = 2 \int_0^h \int_0^{x_1} f(x_1) f(x_2) K_1(x_1, x_2) \, \mathrm{d}x_2 \, \mathrm{d}x_1 U_1 \\ + 2 \int_0^h \int_0^{x_1} f(x_1) f(x_2) K_2(x_1, x_2) \, \mathrm{d}x_2 \, \mathrm{d}x_1 U_2, \end{aligned} \tag{5.2}$$

where

$$K_1(x, y) = \sin \omega(x - y) - \sin \omega x + \sin \omega y, \qquad K_2(x, y) = \cos \omega x - \cos \omega y.$$

Endeavouring to approximate the two integrals in (5.2), we follow the same rules of engagement as in (Iserles et al. 2000): thus, it is permitted to reuse the values of f that have been already evaluated for the quadrature of the univariate integral, and nothing else. Assume for simplicity that $\kappa = \frac{1}{2}$, hence $f(\frac{1}{2}h) = 0$ and the function $\bar{f}(x) = f(x)/(x - \frac{1}{2}h)$ is smooth. The quadratures in the sequel use only function values at the endpoints and, implicitly, rely on $f(\frac{1}{2}h) = 0$: the information from remaining two nodes in (5.1) is discarded. We commence from the first integral. Letting

$$I_h[\bar{f}_1, \bar{f}_2] = \int_0^h \int_0^{x_1} (x_1 - \tfrac{1}{2}h)(x_2 - \tfrac{1}{2}h) \bar{f}_1(x_1) \bar{f}_2(x_2) K_1(x_1, x_2) \, \mathrm{d}x_2 \, \mathrm{d}x_1,$$

it is possible to prove, e.g. by symbolic computation, that

$$I_h[\bar{f}_1, \bar{f}_2] = -\tfrac{1}{3360} f(0) g(0) \omega^3 h^7 + \mathcal{O}\big(h^8\big),$$

therefore nominally the integral can be discarded, being consistent with order six. This, however, disregards the effect of high oscillation: as $\psi = h\omega$ becomes large, the asymptotic expansion is

$$I_h[\bar{f}_1, \bar{f}_2] \sim \tfrac{1}{12} \frac{f(0) g(0) h^4}{\psi} + \mathcal{O}\big(h^5 \psi^{-1}, h^4 \psi^{-2}\big).$$

The prudent course of action, thus, is to retain the integral and replace it by quadrature. To this end, we seek coefficients $\beta_{1,1}, \beta_{1,2}, \beta_{2,1}$ and $\beta_{2,2}$ so that

$$Q_h[\bar{f}_1, \bar{f}_2] = 2h^2 \sum_{k=1}^{2} \sum_{l=1}^{2} \beta_{k,l} f_k(\tilde{c}_k h) f_l(\tilde{c}_l h), \tag{5.3}$$

where $\tilde{c}_1 = 0$, $\tilde{c}_2 = 1$, matches $I_h[\bar{f}_1, \bar{f}_2]$ for (a) $f_1(x) = f_2(x) = x - \frac{1}{2}$; (b) $f_1(x) = x(x - \frac{1}{2})$, $f_2(x) = x - \frac{1}{2}$; (c) $f_1(x) = x - \frac{1}{2}$, $f_2(x) = x(x - \frac{1}{2})$; and (d) $f_1(x) = f_2(x) = x(x - \frac{1}{2})$. As before, the coefficients $\beta_{k,l}$ are allowed to depend on $\psi = h\omega$. Once the weights are known, we set $f_1 = f_2 = f$. Our construction ensures that the quadrature error is $\mathcal{O}\big(h^9\big)$: this, incidentally, is consistent with our decision to use $\nu = 5$ in the univariate quadrature.

We have four linear algebraic equations in four unknowns, whose solution is

$$\begin{aligned}
\beta_{1,1} &= \tfrac{3}{10}\frac{1}{\psi} - \tfrac{1}{6}\frac{\sin\psi}{\psi^2} - \frac{\frac{58}{3}+\frac{5}{3}\cos\psi}{\psi^3} + \frac{13\sin\psi}{\psi^4} + \frac{240+96\cos\psi}{\psi^5} - \frac{336\sin\psi}{\psi^6},\\
\beta_{1,2} &= -\tfrac{1}{30}\frac{1}{\psi} - \tfrac{1}{6}\frac{\sin\psi}{\psi^2} - \frac{\frac{10}{3}+\frac{11}{3}\cos\psi}{\psi^3} + \frac{35\sin\psi}{\psi^4} + \frac{168(1+\cos\psi)}{\psi^5} - \frac{336\sin\psi}{\psi^6},\\
\beta_{2,1} &= \frac{\frac{2}{15}+\frac{1}{6}\cos\psi}{\psi} - \tfrac{3}{2}\frac{\sin\psi}{\psi^2} - \frac{\frac{16}{3}+\frac{29}{3}\cos\psi}{\psi^3} + \frac{51\sin\psi}{\psi^4} + \frac{152+184\cos\psi}{\psi^5}\\
&\quad - \frac{336\sin\psi}{\psi^6},\\
\beta_{2,2} &= \frac{\frac{2}{15}+\frac{1}{6}\cos\psi}{\psi} - \tfrac{5}{2}\frac{\sin\psi}{\psi^2} - \frac{\frac{4}{3}+\frac{59}{3}\cos\psi}{\psi^3} + \frac{93\sin\psi}{\psi^4} + \frac{80+256\cos\psi}{\psi^5} - \frac{336\sin\psi}{\psi^6}.
\end{aligned}$$

Substitution into (5.3) and letting $f_1 = f_2 = f$ results in an order-eight quadrature, with error terms

$$\tfrac{1}{24192}\omega^3 h^9 f(0)f''(0) + \mathcal{O}\big(h^{10}\big) \quad \text{and} \quad \tfrac{1}{120}\frac{h^6 f(0)f''(0)}{\psi} + \mathcal{O}\big(h^7\psi^{-1}, h^6\psi^{-2}\big)$$

for $h \to 0$ and $\psi \to \infty$ respectively. Note that $\beta_{k,l}(\psi) = \mathcal{O}\big(\psi^{-1}\big)$ and $U_1 = \mathcal{O}\big(\psi^{-1}\big)$ imply that the quadrature error for the double integral indeed decays like $\mathcal{O}\big(\psi^{-2}\big)$, consistently with the error for the first, univariate integral.

Next, we deal with the second integral. Note that it can be easily confirmed, e.g. with a symbolic calculator, that its leading terms are

$$\tfrac{1}{240}\omega^2 h^6 f(0)g(0) \qquad \text{and} \qquad \tfrac{1}{24}f(0)g'(0)h^5\frac{\sin\psi}{\psi}$$

for $h \to 0$ and $\psi \to \infty$ respectively. Replacing K_1 with K_2 we obtain in (5.3) the coefficients

$$\begin{aligned}
\beta_{1,1} &= \frac{-\frac{5}{2}+\frac{1}{6}\cos\psi}{\psi^2} - \tfrac{2}{3}\frac{\sin\psi}{\psi^3} + \frac{86-6\cos\psi}{\psi^4} + \frac{80\sin\psi}{\psi^5} - \frac{320(1-\cos\psi)}{\psi^6},\\
\beta_{1,2} &= -\frac{\frac{1}{6}(1-\cos\psi)}{\psi^2} - \tfrac{11}{3}\frac{\sin\psi}{\psi^3} + \frac{34(1-\cos\psi)}{\psi^4} + \frac{160\sin\psi}{\psi^5} - \frac{320(1-\cos\psi)}{\psi^6},\\
\beta_{2.1} &= \tfrac{1}{6}\frac{\sin\psi}{\psi} - \frac{\frac{1}{2}(1-\cos\psi)}{\psi^2} - \tfrac{11}{3}\frac{\sin\psi}{\psi^3} + \frac{34(1-\cos\psi)}{\psi^4} + \frac{160\sin\psi}{\psi^5}\\
&\quad - \frac{320(1-\cos\psi)}{\psi^6},\\
\beta_{2,2} &= \tfrac{1}{6}\frac{\sin\psi}{\psi} - \frac{\frac{1}{6}-\frac{5}{2}\cos\psi}{\psi^2} - \tfrac{56}{3}\frac{\sin\psi}{\psi^3} + \frac{6-86\cos\psi}{\psi^4} + \frac{240\sin\psi}{\psi^5} - \frac{320(1-\cos\psi)}{\psi^6}.
\end{aligned}$$

The quadrature error is

$$-\tfrac{1}{2240}\omega^2 h^8 f(0)f''(0) + \mathcal{O}\big(h^9\big), \qquad h \to 0,$$

and the asymptotic error

$$-\tfrac{1}{24}h^7 f'(0)f''(0)\frac{1+\cos\psi}{\psi^2} + \mathcal{O}\big(h^8\psi^{-2}, h^7\psi^{-3}\big), \qquad \psi \to \infty.$$

In tandem with U_2, this yields error attenuation of $\mathcal{O}(\psi^{-4})$. Note that the order of this quadrature is one less than that for the univariate integral and the first double integral. Of course, we could have increased the order by using additionally the function evaluations at $(\frac{1}{2} \pm \frac{\sqrt{21}}{14})h$ from (5.1), but this is hardly necessary, given that the order of modified Magnus with exact integrals is six, and also since the decay of the error for large ψ is bound to be almost instantaneous, due to the asymptotic error attenuation.

This approach should lend itself to quadrature for higher-order modified Magnus methods, incorporating more integrals. General theory of such multivariate quadrature with highly-oscillatory kernels is a matter for a different paper, hopefully by a different author.

Acknowledgements

The author is indebted to many colleagues who shared their expertise on numerical quadrature and acted as a sounding board for the ideas in this paper, in particular to Brad Baxter, Ilan Degani, Nira Dyn, Walter Gautschi, David Levin, Nick Trefethen and Jeremy Schiff.

References

Bakhvalov, N. S. & Vasilčeva, L. G. (1968), 'Evaluation of the integrals of oscillating functions by interpolation at nodes of Gaussian quadrature', *USSR Comp. & Math. Phys.* **8**, 241–249.

Clendenin, W. W. (1966), 'A method for numerical calculation of Fourier integrals', *Numerische Mathematik* **8**, 422–436.

Davis, P. J. & Rabinowitz, P. (1980), *Methods of Numerical Integration*, 2nd edn, Academic Press, Orlando, FL.

Engels, H. (1980), *Numerical Quadrature and Cubature*, Academic Press, London.

Evans, G. A. & Chung, K. C. (2003), 'Theoretical aspects of generalised quadrature methods', *J. Complexity* **19**, 272–285.

Filon, L. N. G. (1928), 'On a quadrature formula for trigonometric integrals', *Proc. Royal Soc. Edinburgh* **49**, 38–47.

Flinn, E. A. (1960), 'A modification of Filon's method of numerical integration', *J ACM* **7**, 181–184.

Fosdick, L. D. (1968), 'A special case of the Filon quadrature formula', *Maths Comp.* **22**, 77–81.

Gautschi, W. (1968), 'Construction of Gauss–Christoffel quadrature formulas', *Maths Comp.* **22**, 251–270.

Gautschi, W. (1981), A survey of Gauss–Christoffel quadrature formulæ, *in* P. Butzer & F. Fehér, eds, 'E.B. Christoffel. The Influence of His Work on Mathematics and the Physical Sciences', Birkhäuser Verlag, Basel, pp. 72–147.

Goldberg, R. R. & Varga, R. S. (1956), 'Moebius inversion of Fourier transforms', *Duke Math. J.* **23**, 553–559.

Hairer, E., Nørsett, S. P. & Wanner, G. (1993), *Solving Ordinary Differential Equations I: Nonstiff Problems*, 2nd revised edn, Springer Verlag, Berlin.

Iserles, A. (2002*a*), 'On the global error of discretization methods for highly-oscillatory ordinary differential equations', *BIT* **42**, 561–599.

Iserles, A. (2002*b*), 'Think globally, act locally: Solving highly-oscillatory ordinary differential equations', *Appld Num. Anal.* **43**, 145–160.

Iserles, A., Munthe-Kaas, H. Z., Nørsett, S. P. & Zanna, A. (2000), 'Lie-group methods', *Acta Numerica* **9**, 215–365.

Levin, D. (1982), 'Procedure for computing one- and two-dimensional integrals of functions with rapid irregular oscillations', *Maths Comp.* **38**, 531–538.

Levin, D. (1996), 'Fast integration of rapidly oscillatory functions', *J. Comput. Appl. Maths* **67**, 95–101.

Levin, D. (1997), 'Analysis of a collocation method for integrating rapidly oscillatory functions', *J. Comput. Appl. Maths* **78**, 131–138.

Levin, D., Reichel, L. & Ringhoffer, C. (1984), Analysis of an integration method for rapidly oscillating integrands, Technical Report MRC 2670, University of Wisconsin, Madison.

Luke, Y. L. (1954), 'On the computation of oscillatory integrals', *Proc. Cambridge Phil. Soc.* **50**, 269–277.

Lyness, J. N. (1971), 'Adjusted forms of the Fourier coefficient asymptotic expansion and applications in numerical quadrature', *Maths Comp.* **25**, 87–104.

Zamfirescu, I. (1963), 'An extension of Gauss's method for the calculation of improper integrals', *Acad. R.P. Romîne Stud. Cerc. Mat.* **14**, 615–631. (in Romanian).