Three stories of high oscillation

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1 Think globally, act globally!

Numerical analysis – indeed, mathematical analysis – is in large measure a story of the local. Sufficiently smooth functions are approximated very well in a small neighbourhood by polynomials, indeed even by linear functions. A case in point is the granddaddy of all discretisation methods for differential equations, the *Euler method:* given the ordinary differential system $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ and having already found $\boldsymbol{y}_n \approx \boldsymbol{y}(t_n)$, we approximate $\boldsymbol{y}(t_{n+1})$, where $t_{n+1} = y_n + h$, by $\boldsymbol{y}_n + h\boldsymbol{f}(t_n, \boldsymbol{y}_n)$. In other words, we progress from t_n to t_{n+1} assuming that locally the solution is linear, uniquely determined from its value and its slope at t_n. As long as $\boldsymbol{f}$ is twice smoothly differentiable, the error is $O\left(h^2\right)$ and it can be made sufficiently small by choosing small step-size $h > 0$. Of course, in place of linear functions, we can use polynomials, say, or rational functions of increasing degree of sophistication and intricacy but the same principle applies: we zoom on a sufficiently small neighbourhood. *Reductio ad absurdum* of numerical analysis would leave us with a single phrase, "the Taylor theorem".

As long as functions are 'nice', the Taylor theorem is a reasonable foundation stone to numerical algorithms. It is difficult to imagine the modern world without scientific computing and its many achievements: acting locally to think globally is the right strategy most of the time. Yet, important exceptions abound and they come in two flavours. Some functions are not sufficiently smooth to be approximated well by, say, polynomials, calling for more subtle forms of discretisation. Other functions might be misleadingly 'nice', yet their derivatives are large, rendering their local approximation with the Taylor theorem very poor indeed. This is in particular the case with *highly oscillating functions* because, once Taylor series are truncated, the error scales like a (high) derivative but, each time we differentiate, the amplitude is multiplied by frequency.

An accessible example is provided by the *Airy equation* $y'' + ty = 0$. The solution behaves for large t as $y(t) \sim ct^{-1/4} \sin(\frac{2}{3}t^{3/2})$ – it oscillates increasingly fast as t grows [13]. It is easy to confirm that $y^{(m)}(t) \sim ct^{m/2-1/4} \sin(\frac{2}{3}t^{3/2})$, $m \geq 0$, and the amplitude of derivatives increases rapidly for $t \gg 1$. This is demonstrated in Fig. 1.1. Thus, as t grows, $y(t)$ is poorly approximated by polynomials and increasing the polynomial degree actually makes things worse!

High oscillation is present in a very wide range of phenomena and numerical modelling of high-frequency phenomena is vital. Yet, the Taylor theorem alone is inadequate for this purpose, calling for an entirely new breed of discretisation methods. One such type of methods endeavours to bring together numerical analysis and asymptotic expansions, marrying local behaviour with global features of the solution. Three such scenarios are described in this paper: the computation of highly oscillatory integrals, the discretisation of ordinary differential equations with highly oscillatory forcing terms and the computation of the linear Schrödinger equation. In none of the cases have we tried to achieve the greatest possible generality or sophistication, opting instead for accessible examples of numerical methods where global behaviour informs computation.

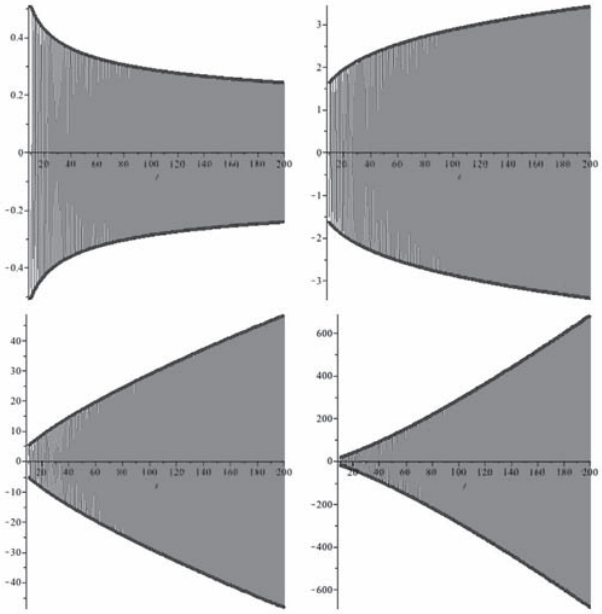

Figure 1.1. The solution of $y'' + ty = 0$, $y(0) = 1$, $y'(0) = 0$ and its first, second and third derivatives. The thick black line depicts the envelope $\pm 0.91 t^{m/2-1/4}$.

2 Story 1: Highly oscillatory quadrature

Computing integrals is an art as old as integration itself and the oldest quadrature method is due to Sir Isaac Newton (although, in fairness to Archimedes, he used something very much like quadrature to calculate the area of a disc). This is the lore of undergraduate numerical analysis courses: given a weight function $w(x) \geq 0$, not identically zero, and assuming that everything in sight is smooth,

$$\int_{a_-}^{a_+} f(x)w(x)\,\mathrm{d}x \approx Q_\nu[f] = \sum_{m=1}^{\nu} b_m f(c_m),$$

where the *nodes* $c_1, \ldots, c_\nu$ are distinct numbers in $[a_-, a_+]$, while $b_1, \ldots, b_\nu$ are the quadrature *weights.* Other things being equal, the best nodes are the zeros of the ν-degree orthogonal polynomial with respect to the L_2 inner product generated by the weight function w and the outcome, *Gaussian quadrature,* is exact for all polynomials f of degree $\leq 2\nu - 1$.

Let

$$I[f](\omega) = \int_{-1}^{1} f(x)\mathrm{e}^{\mathrm{i}\omega x}\,\mathrm{d}x. \tag{2.1}$$

Once ω becomes large, the integrand in (2.1) oscillates at an

increasingly faster pace. In Fig. 2.2 we display the magnitude of the error once Gaussian quadrature is applied to $I[f](\omega)$ for $0 \le \omega \le 50$. The pattern is plain to see. For small ω Gaussian quadrature performs very well and delivers remarkable accuracy: the larger ν, the better. However, once ω grows, roughly when $\omega\nu > 1$, accuracy drops sharply and, after a short while, (2.1) fails to deliver even a single significant digit!

The reason is plain to see: the integrand in (2.1) is very poorly approximated by polynomials of reasonable degree. We are precisely in the regime where the Taylor theorem is of little use! Thus, we turn to asymptotics for help. It is easy to prove that

$$I[f](\omega) \sim -\sum_{n=0}^{\infty} \frac{1}{(-\mathrm{i}\omega)^{n+1}}[f^{(n)}(1)\mathrm{e}^{\mathrm{i}\omega} - f^{(n)}(-1)\mathrm{e}^{-\mathrm{i}\omega}], \quad \omega \gg 1,$$

and this indicates the *asymptotic method*

$$A_s[f](\omega) = -\sum_{n=0}^{s} \frac{1}{(-\mathrm{i}\omega)^{n+1}}[f^{(n)}(1)\mathrm{e}^{\mathrm{i}\omega} - f^{(n)}(-1)\mathrm{e}^{-\mathrm{i}\omega}] \quad (2.2)$$

[9]. Note that the error, $O\left(\omega^{-s-2}\right)$, improves for increasing ω!

Fig. 2.3 on the left displays the error (in a format identical to Fig. 2.2) incurred by (2.2) for $s = 0, 1, 2, 3$, except that we have taken a much larger range of ω. The comparison with Gaussian quadrature is striking: for large ω we require *much* less information, yet obtain a surprisingly precise answer. The *quid pro quo* is that, having committed all our assets to recover 'large ω' behaviour, we can hardly complain that the asymptotic method is useless for small $\omega > 0$. In a sense, Gaussian quadrature and the asymptotic method are complementary.

Which brings us to the right side of Fig. 2.3. We see there for large ω behaviour somewhat better than (2.2) but careful examination of the neighbourhood of the origin indicates that the mystery method performs well also for small ω. Since the extra expense of the mystery method, compared with (2.2), is marginal, we indeed enjoy the best of all worlds: an asymptotic–numerical method.

So, what is the mystery method? Given the nodes $c_1 = -1 < c_2 < \cdots < c_{\nu-1} < c_\nu = 1$, each c_k with a *multiplicity* $m_k \ge 1$, there exists a unique *Hermite interpolating polynomial* p of degree $\sum m_k - 1$ such that $p^{(i)}(c_k) = f^{(i)}(c_k)$, $i = 0, \ldots, m_k - 1$, $k = 1, \ldots, \nu$. A *Filon-type method* consists of replacing f by p in the integral,

$$F_{\boldsymbol{c},\boldsymbol{m}}[f](\omega) = I[p](\omega). \quad (2.3)$$

Let $s = \min\{m_1, m_\nu\}$. It is trivial, substituting $F_{\boldsymbol{c},\boldsymbol{m}}[f] - I[f] = I[p - f]$ into (2.2), to verify that the error is $O\left(\omega^{-s-2}\right)$ [9]: for large ω the behaviour is determined by asymptotics. On the other hand, once $\omega \to 0$, (2.3) collapses into a quadrature method (using both the values of f and of its derivatives) of the classical kind.

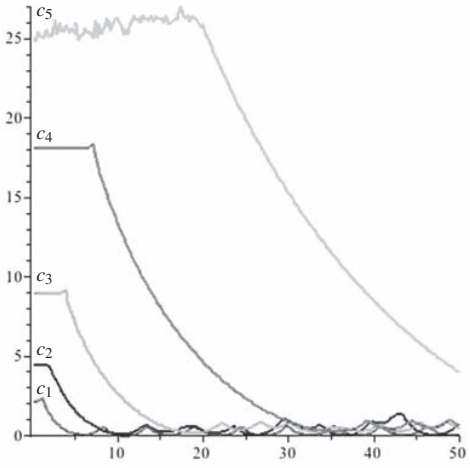

Figure 2.2. The number of significant digits, $-\log_{10}|Q_\nu[f] - I[f]|$, for $f(x) = (2+x)^{-1}$, $\nu = 2$ (c_1), 4 (c_2), 8 (c_3), 16 (c_4) and 32 (c_5) for increasing ω.

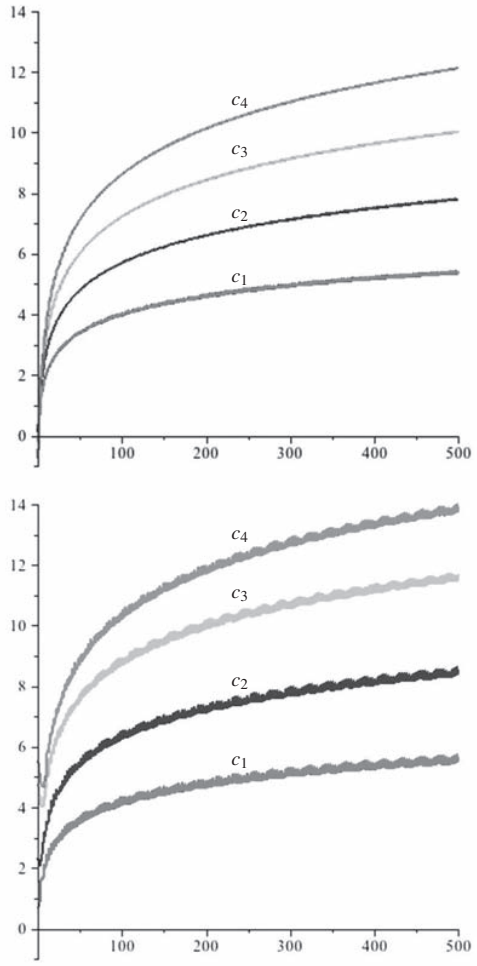

Figure 2.3. The number of significant digits once we use highly oscillatory quadrature. At the top the asymptotic method $A_s[f]$ for $s = 0$ (c_1), 1 (c_2), 2 (c_3) and 3 (c_4). At the bottom the Filon-type method $F_{\boldsymbol{c},\boldsymbol{m}}[f]$ with $\boldsymbol{c} = [-1, 1]$, $\boldsymbol{m} = [1, 1]$ (c_1), $\boldsymbol{c} = [-1, 0, 1]$, $\boldsymbol{m} = [2, 1, 2]$ (c_2), $\boldsymbol{c} = [-1, -1/\sqrt{3}, 0, 1/\sqrt{3}, 1]$, $\boldsymbol{m} = [3, 1, 1, 1, 3]$ (c_3) and $\boldsymbol{c} = [-1, -\sqrt{3/11}, 0, \sqrt{3/11}, 1]$, $\boldsymbol{m} = [4, 1, 1, 1, 4]$ (c_4).

Beyond Filon-type methods. It is easy to extend the Filon method to integrals of the kind

$$\int_{a_-}^{a_+} f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\,\mathrm{d}x,$$

provided that $g' \ne 0$ in $[a_-, a_+]$. More effort is required to deal with the case of stationary points $\xi \in [a_-, a_+]$ where $g'(\xi) = 0$. In that case we need to interpolate to f and a suitable number of derivatives at

stationary points to recover the asymptotic behaviour of the 'plain' Filon-type method [9]. All this extends to a multivariate setting [10].

However, Filon-type methods are just one of the new breed of highly oscillatory quadrature methods, alongside Levin methods [12, 14] and the numerical stationary phase method [8]. The last word is a methodology which combines an insight from both Filon-type and stationary phase approaches in a true tour de force of asymptotics-cum-numerics [7].

3 Story 2: A highly oscillatory forcing term

A good starting point is the differential equation for a nonlinear, frictionless pendulum which, in dimensionless form, reads $y'' + \sin y = 0$, $y(0) = y_0$, $y'(0) = y'_0$. This is a Hamiltonian system in a single variable and its dynamics is as simple as they come: the origin is a centre, surrounded in the phase plane by stable periodic orbits. Suppose, however, that we impart rapid oscillations to the base of the pendulum: the outcome is the non-autonomous equation

$$y'' + \sin y = c\cos\omega t, \quad t \geq 0, \quad y(0) = y_0, \quad y'(0) = y'_0, \tag{3.4}$$

where $\omega \gg 1$. What can we expect from the solutions of (3.4)? Fig. 3.4 displays a trajectory corresponding to $y_0 = 2$, $y'_0 = 0$ and $c = 1$ in the phase plane for $\omega = 5, 10$ and 20. We can discern a black curve in the background: this is the corresponding trajectory of the nonlinear pendulum $y'' + \sin y = 0$ and it is evident that the trajectory of the forced equation winds round and round the periodic trajectory of the unforced equation. Surprisingly, the amplitude of this winding motion *decreases* with ω. (This is the reason why we have used in Fig. 3.4 such modest values of ω: with much greater values the winding motion would have been invisible to the naked eye.)

This effect of growing ω is important: rapid oscillation of the forcing term leads to an increasingly smaller perturbation and it stabilises the motion. By the same token, slowing down the oscillation destabilises the motion: try the same computation with $\omega = 2$. There is an important lesson here: high oscillation is good for dynamics while, at the same time, being lethal for naive numerics. True to our paradigm, instead of relying on the (local) Taylor series, we seek an asymptotic expansion.

It is convenient to consider a broader framework: following [3], we examine the equation

$$y''+f(y) = \sum_{m=-\infty}^{\infty} a_m(t)\mathrm{e}^{\mathrm{i}m\omega t}, \quad t \geq 0, \quad y(0) = y_0, \quad y'(0) = y'_0, \tag{3.5}$$

where f and a_m, $m \in \mathbb{Z}$, are analytic functions and $\sum_m |a_m(t)| < \infty$, $t \geq 0$. Our claim is that we can expand the solution in the form

$$y(t) \sim p_{0,0}(t) + \sum_{r=2}^{\infty} \frac{1}{\omega^r} \sum_{m=-\infty}^{\infty} p_{r,m}(t)\mathrm{e}^{\mathrm{i}m\omega t}, \qquad t \geq 0, \tag{3.6}$$

where the functions $p_{r,m}$, which are independent of ω, can be obtained explicitly in a recursive manner.

In principle, we need to expand everything in (3.5) in asymptotic series. This is fairly easy for $y''(t)$ but much more challenging (and messy) for $f(y(t))$ and, at the conclusion of all this algebra galore, we have an expansion in two scales: *orders of magnitude* ω^{-r} and *oscillators* $\mathrm{e}^{\mathrm{i}m\omega t}$. We commence by

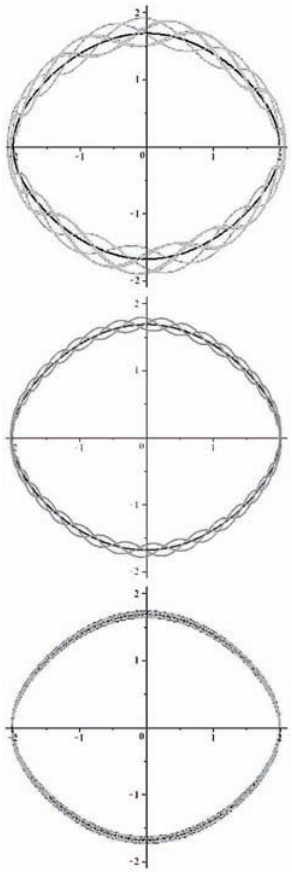

Figure 3.4. A phase-plane trajectory of the solution of $y'' + \sin y = \cos\omega t$, $y(0) = 3$, $y'(0) = 0$, with $\omega = 5, 10, 20$. The black curve is the corresponding periodic trajectory of $y'' + \sin y = 0$.

separating the expansion into orders of magnitude. For $r = 0$ we have

$$p''_{0,0} - \sum_{m=-\infty}^{\infty} m^2 p_{2,m}\mathrm{e}^{\mathrm{i}m\omega t} + f(p_{0,0}) = \sum_{m=-\infty}^{\infty} a_m\mathrm{e}^{\mathrm{i}m\omega t}$$

and, separating oscillators, we have

$$p''_{0,0} + f(p_{0,0}) = 0, \quad t \geq 0, \qquad p_{0,0}(0) = y_0, \quad p'_{0,0}(0) = y'_0,$$
$$p_{2,m} = -\frac{a_m}{m^2}, \qquad m \neq 0. \tag{3.7}$$

Note that we have imposed on $p_{0,0}$ the same initial conditions as on y; this means that we need to impose $\sum_m p_{r,m}(0) = \sum_m p'_{r,m}(0) = 0$ in the sequel.

Next, over to $r = 1$,

$$\sum_{m=-\infty}^{\infty} (2\mathrm{i}mp'_{2,m} - m^2 p_{3,m})\mathrm{e}^{\mathrm{i}m\omega t} = 0$$

and, separating scales,

$$p_{3,m} = \frac{2\mathrm{i}}{m}p'_{2,m} = -\frac{2\mathrm{i}}{m^3}a'_m, \qquad m \neq 0. \tag{3.8}$$

Likewise, $r = 2$ results in

$$\sum_{m=-\infty}^{\infty} (p''_{2,m} - 2\mathrm{i}mp'_{3,m} - m^2 p_{4,m})\mathrm{e}^{\mathrm{i}m\omega t} + f'(p_{0,0}) \sum_{m=-\infty}^{\infty} p_{2,m}\mathrm{e}^{\mathrm{i}m\omega t} = 0,$$

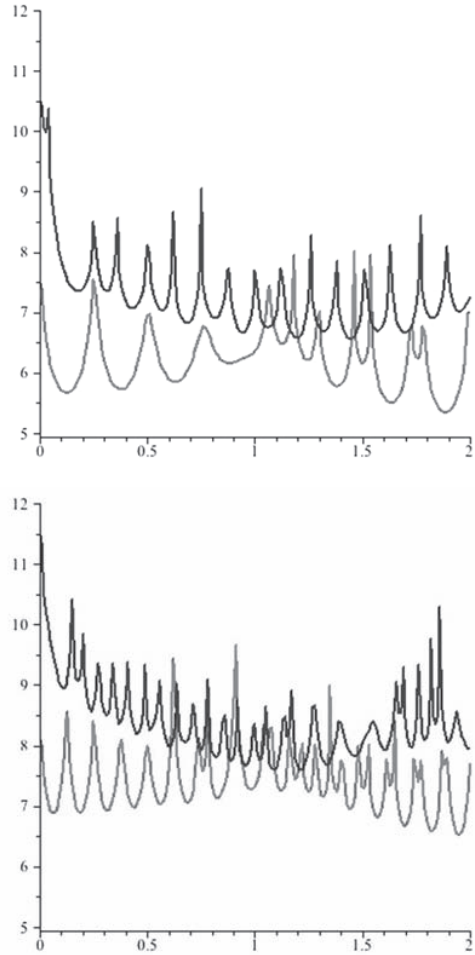

Figure 3.5. The error $-\log_{10}|y^{[s]}(t)-y(t)|$ **for the forced nonlinear pendulum (3.4):** $\omega = 25$ **at the top and** $\omega = 50$ **at the bottom,** $s = 2$ **in gray and** $s = 4$ **in black.**

therefore

$$\begin{aligned} p''_{2,0} + f'(p_{0,0})p_{2,0} = 0, \quad t \ge 0, \\ \sum_{m=-\infty}^{\infty} p_{2,m}(0) = \sum_{m=-\infty}^{\infty} p'_{2,m}(0) = 0, \\ p_{4,m} = \frac{1}{m^2}[p''_{2,m} - 2\mathrm{i}mp'_{3,m} + f'(p_{0,0})p_{2,m}], \\ m \ne 0. \end{aligned} \tag{3.9}$$

A general rule emerges: for each order of magnitude r we obtain $p_{r,0}$ solving a differential equation and $p_{r+2,m}$, $m \ne 0$, by recursion. These differential equations need to be solved numerically but this is not a problem since they are all non-oscillatory: the solution becomes oscillatory only once we assemble it into an appropriately truncated expansion (3.6),

$$y^{[s]}(t) = p_{0,0}(t) + \sum_{r=2}^{s} \frac{1}{\omega^r} \sum_{m=-\infty}^{\infty} p_{r,m}(t)\mathrm{e}^{\mathrm{i}m\omega t}, \qquad t \ge 0.$$

All relevant equations can be derived explicitly [3].

Specialising to the forced nonlinear pendulum (3.4), we use (3.4–6) and, for good measure, consider also $r = 3, 4$. We have $p_{3,m} \equiv 0$,

$$\begin{aligned} p''_{0,0} + \sin p_{0,0} = 0, \quad t \ge 0, \\ p_{0,0}(0) = 2, \quad p'_{0,0}(0) = 0, \\ p''_{2,0} + (\cos p_{0,0})p_{2,0} = 0, \quad t \ge 0, \\ p_{2,0}(0) = 1, \quad p'_{2,0}(0) = 0, \\ p''_{4,0} + (\cos p_{0,0})p_{4,0} = \tfrac{1}{4}(1 + 2p_{0,0}^2)\sin p_{0,0}, \\ p_{4,0}(0) = \cos 2, \quad p'_{4,0}(0) = 0, \end{aligned}$$

and

$$\begin{aligned} y^{[2]}(t) &= p_{0,0}(t) + \frac{1}{\omega^2}[p_{2,0}(t) - \cos\omega t], \\ y^{[4]}(t) &= p_{0,0}(t) + \frac{1}{\omega^2}[p_{2,0}(t) - \cos\omega t] \\ &\quad + \frac{1}{\omega^4}[p_{4,0}(t) - \cos\omega t \cos p_{0,0}(t)]. \end{aligned}$$

Fig. 3.5 displays the number of significant digits recovered by $y^{[2]}$ and $y^{[4]}$, respectively, for $\omega = 25$ and $\omega = 50$. All is in line with the theory and if the accuracy is insufficient for you – well, just take larger ω ...

Beyond highly oscillatory forced ODEs. Equation (3.5) is but one example of ordinary differential equations with highly oscillatory forcing which can be expanded by this synthesis of asymptotic and numerical reasoning. With greater generality, it is possible to extend this analysis to ODE systems

$$\boldsymbol{y}' = \boldsymbol{f}(\boldsymbol{y}) + \sum_{m=-\infty}^{\infty} \boldsymbol{a}_m(t)\mathrm{e}^{\mathrm{i}m\omega t}, \quad t \ge 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0$$

[4, 15] and beyond. Equations of this kind are important in many applications, e.g., in electronics, where oscillation is generated by high-frequency input.

A more general framework is provided by the *heterogeneous multi scale method* [1] and it allows not just highly oscillatory forcing terms but also highly oscillatory coefficients, but the *quid pro quo* is that expansions can be practically generated up to $O(\omega^{-r})$ only for fairly modest values of $r \ge 1$.

4 Story 3: The linear Schrödinger equation

The *linear Schrödinger equation*

$$\partial_t u = \mathrm{i}\varepsilon\partial_x^2 u + \mathrm{i}\varepsilon^{-1}V(x)u, \qquad t \ge 0, \quad -1 \le x \le 1, \tag{4.10}$$

where both the initial value $u(\,\cdot\,, 0)$ and the *interaction potential* $V(x)$ are smooth and periodic, describes the quantum state of a single particle: essentially, it is the equivalent of Newton's law in a quantum setting. The parameter $\varepsilon > 0$ is very small, rendering the solution of this deceptively simple linear PDE fairly knotty.

Standard numerical wisdom goes along the following lines: we commence by discretising (4.10) in some M-dimensional space, e.g., by replacing $\partial_x^2 u$ by a linear combination of function values along a grid (finite differences) or moving to Fourier space and considering there an L_2 projection on Nth degree trigonometric polynomials, $M = 2N + 1$ (a spectral method). The outcome is a set of linear ODEs of the form

$$\boldsymbol{u}' = \mathrm{i}(\varepsilon\mathcal{K} + \varepsilon^{-1}\mathcal{D}_V)\boldsymbol{u}, \quad t \ge 0, \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0, \tag{4.11}$$

where $\mathcal{K}$ and $\mathcal{D}_V$ are matrices corresponding to approximate differentiation and multiplication by V, respectively. Solving

(4.11) should be easy in principle; after all an explicit solution is available,

$$\boldsymbol{u}(t) = \exp\left(\mathrm{i}t(\varepsilon\mathcal{K} + \varepsilon^{-1}\mathcal{D}_V)\right)\boldsymbol{u}_0, \qquad t \geq 0,$$

except that the tiny ε spoils the party. The dimension M is large (and our real interest is in considering (4.10) in a multivariate setting: the dimension soon becomes *really* large!) and the only realistic hope of computing the matrix exponential with reasonable accuracy is by *Krylov subspace methods* [6]: we replace the computation of a 'big' exponential by a (hopefully) small, $m \times m$, one, at a cost of $O\left(m^2M\right)$ operations. Except that our hope is in vain: once ε is very small, m becomes large, $m = O(M)$, and the overall cost, $O\left(M^3\right)$, is unacceptably large.

The good news is that a ready alternative is available: an *exponential splitting*. In its simplest manifestation, the *Strang splitting*

$$\mathrm{e}^{\mathrm{i}t(\varepsilon\mathcal{K}+\varepsilon^{-1}\mathcal{D}_V)} \approx \mathrm{e}^{\frac{1}{2}\mathrm{i}t\varepsilon\mathcal{K}}\mathrm{e}^{\mathrm{i}t\varepsilon^{-1}\mathcal{D}_V}\mathrm{e}^{\frac{1}{2}\mathrm{i}t\varepsilon\mathcal{K}} \tag{4.12}$$

incurs an error of $O\left(t^3\right)$ and is easy to evaluate: e.g., once we use a spectral method, $\mathcal{K}$ is a diagonal matrix and $\mathcal{D}_V$ a circulant, whose exponential can be evaluated with two Fast Fourier Transforms (FFT) [11]. Unfortunately, the error $O\left(t^3\right)$ of the Strang splitting is unacceptably large.

It is possible to design higher-order splittings, e.g.

$$\mathrm{e}^{\frac{1}{2}\alpha t\mathcal{B}}\mathrm{e}^{\alpha t\mathcal{A}}\mathrm{e}^{\frac{1}{2}(1-\alpha)t\mathcal{B}}\mathrm{e}^{(1-2\alpha)t\mathcal{A}}\mathrm{e}^{\frac{1}{2}(1-\alpha)t\mathcal{B}}\mathrm{e}^{\alpha t\mathcal{A}}\mathrm{e}^{\frac{1}{2}\alpha t\mathcal{B}}, \tag{4.13}$$

where $\mathcal{B} = \mathrm{i}\varepsilon\mathcal{K}$, $\mathcal{A} = \mathrm{i}\varepsilon^{-1}\mathcal{D}_V$ and $\alpha = (2 - \sqrt[3]{2})^{-1}$ has error of $O\left(t^5\right)$. In general, we can get $O\left(t^{2n+1}\right)$ with $2 \cdot 3^{n-1} + 1$ terms but this is simply much too much for practical computation with large n, even though each individual exponential is cheap. Moreover, note that all these are expansions in the step size t but we have two other small quantities, ε and M^{-1}: a good expansion should take them all into account.

By this stage of our narrative, a remedy should stare us in the face: an asymptotic expansion! Following upon the ideas in [2], we thus assume that $t \sim O\left(\varepsilon^{1/2}\right)$, $M \sim O\left(\varepsilon^{-1/2}\right)$ and seek an expansion of the form

$$\mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\cdots\mathrm{e}^{\mathcal{R}_s}\mathrm{e}^{\mathcal{T}_{s+1}}\mathrm{e}^{\mathcal{R}_s}\cdots\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0} \tag{4.14}$$

where $\mathcal{R}_0 = O\left(\varepsilon^{-1/2}\right)$, $\mathcal{R}_1 = O\left(\varepsilon^{1/2}\right)$, $\ldots$, $\mathcal{R}_s = O\left(\varepsilon^{s-1/2}\right)$ and $\mathcal{T}_s = O\left(\varepsilon^{s+1/2}\right)$: an asymptotic splitting.

An important observation with regard to (4.3–5) is that they are all *palindromic:* the same whether we read them from the left or from the right. This has a number of advantages. This time symmetry is good in minimising the number of terms because all expansions are in odd powers of the small parameter. Moreover, since both $\mathrm{i}\partial_x^2$ and multiplication by $\mathrm{i}V$ are skew-Hermitian operators, the solution operator of (4.10) is unitary and palindromy makes it easier to respect this feature under discretisation.

The right approach towards computing the asymptotic splitting (4.14) is to abandon the semi-discretisation (4.11) for the time being and split the formal solution operator, $\exp\left(\mathrm{i}t(\varepsilon\partial_x^2 + \varepsilon^{-1}V)\right)$. Only once we have done so, we replace everything with a finite-dimensional approximation. Our main weapon is the *symmetric Baker–Campbell–Hausdorff (sBCH) formula*

$$\mathrm{e}^{\frac{1}{2}X}\mathrm{e}^{Y}\mathrm{e}^{\frac{1}{2}X} = \mathrm{e}^{\mathrm{sBCH}(X,Y)}$$

where

$$\begin{aligned}\mathrm{sBCH}(tX, tY) = {} & t(X+Y) - t^3(\tfrac{1}{24}[[Y,X],X] + \tfrac{1}{12}[[Y,X],Y]) \\ & + t^5(\tfrac{7}{5760}[[[[Y,X],X],X],X] \\ & + \tfrac{7}{1440}[[[[Y,X],X],X],Y] \\ & + \tfrac{1}{180}[[[[Y,X],X],Y],Y] \\ & + \tfrac{1}{720}[[[[Y,X],Y],Y],Y] \\ & + \tfrac{1}{480}[[[Y,X],X],[Y,X]]) + O\left(t^7\right).\end{aligned}$$

Note that the expansion is in odd powers of t, reaping a benefit of palindromy!

We let $\tau = \mathrm{i}\Delta t$, where Δt is the time step. The algorithm commences by setting $\mathcal{T}_0 = \tau\varepsilon^{-1}V + \tau\varepsilon\partial_x^2$ (the term we wish to split) and $\mathcal{R}_0 = \frac{1}{2}\tau\varepsilon^{-1}V$ (half the asymptotically larger term, which we wish to knock out by this stage), therefore

$$\mathrm{e}^{\tau\varepsilon^{-1}V+\tau\varepsilon\partial_x^2} = \mathrm{e}^{\mathcal{T}_0} = \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathrm{sBCH}(-2\mathcal{R}_0,\mathcal{T}_0)}\mathrm{e}^{\mathcal{R}_0}.$$

Note that, having just 'decapitated' the leading term, $\mathcal{T}_1 := \mathrm{sBCH}(-2\mathcal{R}_0, \mathcal{T}_0) = O\left(\varepsilon^{1/2}\right)$, we next identify the leading (i.e. $O\left(\varepsilon^{1/2}\right)$) term of $\mathcal{T}_1$ and let $\mathcal{R}_1$ be half of it. Therefore

$$\mathrm{e}^{\tau\varepsilon^{-1}V+\tau\varepsilon\partial_x^2} = \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathrm{sBCH}(-2\mathcal{R}_1,\mathcal{T}_1)}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0}$$

and $\mathrm{sBCH}(-2\mathcal{R}_1, \mathcal{T}_1) = O\left(\varepsilon^{3/2}\right)$. We continue in this vein until the right accuracy has been attained, except that, more perhaps than elsewhere, the devil is in the detail! On the face of it, the sBCH formula introduces commutators galore and this might mire the entire enterprise in expensive calculations. Except that, upon further examination, commutators go away! For example, it is easy to confirm that $[V, \partial_x^2] = -V'' - 2V'\partial_x$. In general, every combination of nested commutators of V and ∂_x^2 can be written in the form $\sum_{k=0}^{n} y_k(x)\partial_x^k$ for some $n \geq 0$ and functions $y_1, \ldots, y_n$ which depend on V and its derivatives.

Commutators go away but another problem rears its head: odd powers of ∂_x, which may cause instability and play havoc with our expansions. The remedy is to get rid of odd derivatives by a simple trick, e.g.

$$y(x)\partial_x = -\tfrac{1}{2}\int_{x_0}^{x} y(\xi)\,\mathrm{d}\xi\partial_x^2 - \tfrac{1}{2}y'(x) + \tfrac{1}{2}\partial_x^2\left[\int_{x_0}^{x} y(\xi)\,\mathrm{d}\xi\right].$$

We have only even-order derivative operators on the right and all is well! The outcome,

$$\begin{aligned}\mathcal{R}_0 &= \tfrac{1}{2}\tau\varepsilon^{-1}V = O\left(\varepsilon^{-1/2}\right), \\ \mathcal{R}_1 &= \tfrac{1}{2}\tau\varepsilon\partial_x^2 + \tfrac{1}{24}\tau^3\varepsilon^{-1}V'' = O\left(\varepsilon^{1/2}\right), \\ \mathcal{R}_2 &= -\tfrac{1}{12}\tau^3\varepsilon\{\partial_x^2(V''\,\cdot) + V''\partial_x^2\} + \tfrac{1}{120}\tau^5\varepsilon^{-1}V''V^2 = O\left(\varepsilon^{3/2}\right),\end{aligned}$$

etc. is our asymptotic splitting.

Now – and only now – we discretise derivatives by one of the very powerful methods of numerical analysis, e.g., spectral collocation [5]. All this procedure can be further improved by, paradoxically, first knocking out the *smaller* term $\tau\varepsilon\partial_x^2$ since this counterintuitive step means that all $O\left(\varepsilon^{m/2}\right)$ exponentials for $m \leq \frac{1}{2}$ can be evaluated easily either because they are diagonal or by FFT. The remaining exponentials can be reduced by Krylov subspace methods to a *very* small number of dimensions, e.g., for $s = 2$ we need just dimension 3 for $\mathcal{R}_2$ and dimension 2 for $\mathcal{T}_3$.

Beyond univariate Schrödinger. Equation (4.10) is the simplest model of linear Schrödinger equations in quantum chemistry. In general, we wish to solve the multivariate equation $\partial_t u = \mathrm{i}\varepsilon\nabla^2 u + \mathrm{i}\varepsilon^{-1}V(\boldsymbol{x})u$ in a d-dimensional torus. Provided that d is moderately small, the asymptotic expansion (4.14) generalises and, at the cost of $O\big(N^d \log N\big)$ operations, remains practically feasible. However, once d is large, this approach must be matched by specialised methodologies for highly-dimensional setting, e.g., sparse grids: this is under active research. Another generalisation is to time-dependent interaction potentials, important if magnetism effects are taken on board.

Yet, the potential scope of 'asymptotic splitting' is much wider, not just because of the asymptotic rate of decay but because commutators are replaced by easy-to-evaluate expressions. Only future can tell the limits of this methodology.

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Touching the Abstract: Mathematics at the Museum

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A visitor venturing into the mathematics section of a modern science museum could happen on one of the most interesting, stimulating, surprising mechanical phenomena: a Lorenz chaotic water wheel. Many of you will be familiar with it: water flows into containers that hang on the edge of a rotating circle and slowly leaks from a hole in the bottom. In the beginning, the movement is rather regular and predictable but soon, either because some visitor sneezes or because the jet is not perfectly uniform or because some butterfly flaps its wings in the Amazon jungle, the movement becomes essentially irregular: even a powerful computer cannot predict it for more than a few minutes in advance. In essence, it's a brilliant example of deterministic chaos – a process in which unavoidable perturbations in the environment multiply so quickly that a medium-term forecast is impossible. Still, modern mathematics is able to explain these phenomena: the fountain is a physical model of the power of mathematics and an example of its success.

Science museums haven't always had such spectacular mathematics sections. On the contrary, the oldest ones, especially, seemed to want to reproduce the pedantic approach of school learning: portraits of famous mathematicians of the past hung on the walls of the room; three-dimensional models in display cases showed the interests of 19th century mathematicians; and all around the room