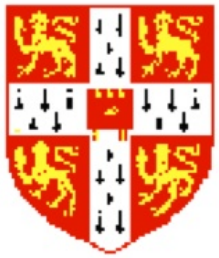

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Part I: Semiclassical Schrödinger

Our point of departure: the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial u}{\partial t} = H(x,t,u)u,$$

where u is the wave function and H the Hamiltonian operator of a quantum system, while $\hbar$ is the Planck constant, divided by 2π.

The Born–Oppenheimer approximation for a non-relativistic particle moving in an electric field results in the Hamiltonian

$$H(x) = -\frac{\hbar^2}{2m}\nabla^2 - V(\boldsymbol{x}),$$

where V is the potential and m is the mass of the particle. This can be generalised to any number of particles.

A semiclassical Schrödinger should not be confused with the nonlinear Schrödinger equation $\mathrm{i}u_t = u_{xx} \pm |u|^2 u$ and its many relatives, neither with the spectral Schrödinger problem $\nabla^2 u + V(\boldsymbol{x})u = \lambda u$.

Zooming on a window of quantum-mechanical significance, we obtain (for simplicity, in 1D)

$$\frac{\partial u}{\partial t} = \mathrm{i}\varepsilon \frac{\partial^2 u}{\partial x^2} + \mathrm{i}\varepsilon^{-1} V(x) u, \qquad x \in [-1, 1],$$

with initial conditions at $t = 0$ and **periodic** boundary conditions at ± 1. Here ε is small, but not *very* small, e.g. $\varepsilon \in [10^{-8}, 10^{-4}]$: typically, it is the square root of the ratio of masses of the smallest particle (an electron!) and the large ones (nuclei). $u(x, t)$ is the position density of a particle.

The equation is difficult because the small parameter generates oscillations at a frequency $\mathcal{O}\left(\varepsilon^{-1}\right)$ – the familiar wavepackets of quantum mechanics.

Structure conservation The L_2 norm of the solution is conserved, i.e. the solution operator is unitary. It is vital that this is preserved under discretisation.

Standard approach

1. Semidiscretise, either with a spectral method or with Hagedorn wavepackets: the outcome is the ODE

$$\boldsymbol{u}' = (\mathrm{i}\varepsilon\mathcal{D} + \mathrm{i}\varepsilon^{-1}\mathcal{V})\boldsymbol{u}, \qquad t \geq 0.$$

2. Compute the solution,

$$\boldsymbol{u}^{n+1} = \mathrm{e}^{\mathrm{i}\Delta t(\varepsilon\mathcal{D}+\varepsilon^{-1}\mathcal{V})}\boldsymbol{u}^n, \qquad n \in \mathbb{Z}_+.$$

Since dimensions are large, the exponential need be approximated, e.g. by Krylov subspace methods. Yet, because of the large ε^{-1}, such methods are totally ineffective. The answer? Exponential splittings.

The Strang splitting: $$\mathrm{e}^{\tau(\varepsilon\mathcal{D}+\varepsilon^{-1}\mathcal{V})} = \mathrm{e}^{\frac{1}{2}\varepsilon\tau\mathcal{D}}\mathrm{e}^{\varepsilon^{-1}\tau\mathcal{V}}\mathrm{e}^{\frac{1}{2}\mathrm{i}\varepsilon\tau\mathcal{D}} + \mathcal{O}\left(\tau^3\right).$$

Note that $\mathrm{e}^{\frac{1}{2}\varepsilon\tau\mathcal{D}}$ and $\mathrm{e}^{\varepsilon^{-1}\tau\mathcal{V}}$ can be typically computed rapidly, either directly or with FFT, and unitarity is preserved.

Problems with the Strang splitting: Low order can be improved e.g. by the Yošida splitting but the number of splittings increases exponentially with the order. Worse, the concept of order is inadequate because we have *three* small parameters: Δt, ε and N^{-1}, where N is the number of spatial degrees of freedom. Unless we want humungous error constants, all three must be taken into account!

Symmetric Zassenhaus splittings (Bader, Al, Kropielnicka & Singh)**:** Don't discretise yet! First let $\Delta t = \mathcal{O}(\varepsilon^\sigma)$, $\sigma > 0$, and $N = \mathcal{O}\Big(\varepsilon^{-1}\Big)$. (Hence $\partial_x = \mathcal{O}\Big(\varepsilon^{-1}\Big)$.) We seek a palindromic expansion

$$\mathrm{e}^{\tau(\varepsilon\partial_x^2+\varepsilon^{-1}V)} \approx \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\dots\mathrm{e}^{\mathcal{R}_s}\mathrm{e}^{\mathcal{T}_{s+1}}\mathrm{e}^{\mathcal{R}_s}\dots\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0},$$

where $\tau = \mathrm{i}\Delta t$, $\mathcal{R}_k = \mathcal{O}(\varepsilon^{\alpha_k})$ where $\alpha_{k+1} \geq \alpha_k$ and $\mathcal{T}_{s+1} = \mathcal{O}(\varepsilon^{\alpha_s+1})$.

Like in Strang's splitting, palindromy ensures that the approximation is unitary.

Deriving Zassenhaus: Set

$$\mathcal{T}_0 = \overbrace{\tau\varepsilon\partial_x^2}^{\mathcal{O}(\varepsilon^{\sigma-1})} + \overbrace{\tau\varepsilon^{-1}V}^{\mathcal{O}(\varepsilon^{\sigma-1})}, \qquad \mathcal{R}_0 = \tfrac{1}{2}\tau\varepsilon^{-1}V.$$

Once we have derived $\mathcal{T}_q = \mathcal{O}(\varepsilon^{\alpha_q})$, set $\mathcal{R}_q$ to half its leading term and

$$\mathrm{e}^{\mathcal{T}_q} = \mathrm{e}^{\mathcal{R}_q}\mathrm{e}^{\mathcal{T}_{q+1}}\mathrm{e}^{\mathcal{R}_q} \;\Rightarrow\; \mathcal{T}_{q+1} = \mathsf{log}\left(\mathrm{e}^{-\mathcal{R}_q}\mathrm{e}^{\mathcal{T}_q}\mathrm{e}^{-\mathcal{R}_q}\right) = \mathsf{sBCH}(-2\mathcal{R}_q, \mathcal{T}_q),$$

where sBCH is the symmetric Baker–Campbell–Hausdorff operator, $\mathrm{e}^{\frac{1}{2}X}\mathrm{e}^{Y}\mathrm{e}^{\frac{1}{2}X} = \mathrm{e}^{\mathsf{sBCH}(X,Y)}$ where

$$\begin{aligned}\mathsf{sBCH}(X,Y) &= (X+Y) - \left(\tfrac{1}{24}[[Y,X],X] + \tfrac{1}{12}[[Y,X],X]\right)\\ &+\Big(\tfrac{7}{5760}[[[[Y,X],X],X],X]+\tfrac{7}{1440}[[[[Y,X],X],X],Y]+\tfrac{1}{180}[[[[Y,X],X],Y],Y]\\ &\quad+\tfrac{1}{720}[[[[Y,X],Y],Y],Y]+\tfrac{1}{480}[[[Y,X],X],[Y,X]]-\tfrac{1}{360}[[[Y,X],Y],[Y,X]]\Big)+\cdots.\end{aligned}$$

Let $\sigma = 1$, i.e. $\Delta t = \mathcal{O}(\varepsilon)$. Then

$$\begin{aligned}\mathcal{T}_1 = &\overbrace{\tau\varepsilon\partial_x^2}^{\mathcal{O}(1)} + \overbrace{\tfrac{1}{12}\tau^3\varepsilon^{-1}(\partial_x V)^2 - \tfrac{1}{2}\tau\varepsilon(\partial_x^2 V)\partial_x^2}^{\mathcal{O}(\varepsilon^2)} - \overbrace{\tfrac{1}{3}\tau^3\varepsilon(\partial_x^3 V)\partial_x}^{\mathcal{O}(\varepsilon^3)} \\ &+ \overbrace{\tfrac{1}{60}\tau^5\varepsilon^{-1}(\partial_x^2 V)(\partial_x V)^2 - \tfrac{1}{12}\tau^3\varepsilon(\partial_x^4 V)}^{\mathcal{O}(\varepsilon^4)} \\ &+ \overbrace{\tau^5\varepsilon\left[\tfrac{4}{45}(\partial_x^2 V)^2 - \tfrac{1}{90}(\partial_x^3)(\partial_x V)\right]\partial_x^2 + \tfrac{1}{45}\tau^5\varepsilon^3(\partial_x^4 V)\partial_x^4}^{\mathcal{O}(\varepsilon^4)} \\ &+ \overbrace{\tau^5\varepsilon\left[\tfrac{1}{6}(\partial_x^3 V)(\partial_x^2 V) - \tfrac{1}{90}(\partial_x^4 V)(\partial_x V)\right]\partial_x}^{\mathcal{O}(\varepsilon^5)} \\ &+ \overbrace{\tfrac{2}{45}\tau^5\varepsilon^3(\partial_x^5 V)\partial_x^3}^{\mathcal{O}(\varepsilon^5)} + \mathcal{O}\left(\varepsilon^6\right)\end{aligned}$$

Except that we have a problem: for unitarity we want $\mathcal{T}_1$ to be skew-Hermitian, but this is inconsistent with the presence of $\mathrm{i}\partial_x^{2k+1}$ in the $\mathcal{O}\left(\varepsilon^3\right)$ and $\mathcal{O}\left(\varepsilon^5\right)$ terms.

Once ∂_x is discretised by a skew-symmetric matrix, $\mathrm{i}\partial_x^{2k}$ becomes a skew-Hermitian matrix: **good!** However, $\mathrm{i}\partial_x^{2k+1}$ becomes Hermitian – **bad!**

Time for a massage! Specifically, given any smooth function U, replace

$$
\begin{aligned}
U\partial_x &= -\tfrac{1}{2}(\partial_x U) - \tfrac{1}{2}\int_0^x U(\xi)\,\mathrm{d}\xi\partial_x^2 + \tfrac{1}{2}\partial_x^2\left[\int_0^x U(\xi)\,\mathrm{d}\xi\,\cdot\right],\\
U\partial_x^3 &= -(\partial_x U)\partial_x^2 - \tfrac{1}{2}\partial_x^2[(\partial_x U)\,\cdot] + \tfrac{1}{4}(\partial_x^3 U)\\
&\qquad - \tfrac{1}{4}\int_0^x U(\xi)\,\mathrm{d}\xi\partial_x^4 + \tfrac{1}{4}\partial_x^4\left[\int_0^x U(\xi)\,\mathrm{d}\xi\,\cdot\right]
\end{aligned}
$$

(and so on): note that there are only even derivatives on the right-hand side!

Following the massage...

$$\mathcal{T}_1 = \overbrace{\tau\varepsilon\partial_x^2}^{\mathcal{O}(1)} + \overbrace{\tfrac{1}{12}\tau^3\varepsilon^{-1}(\partial_x V)^2 - \tfrac{1}{6}\tau^3\varepsilon\{(\partial_x^2 V)\partial_x^2 + \partial_x^2[(\partial_x^2 V)\cdot]\}}^{\mathcal{O}(\varepsilon^2)}$$
$$+ \overbrace{\tfrac{1}{60}\tau^5\varepsilon^{-1}(\partial_x^2 V)(\partial_x V)^2 + \tfrac{1}{12}\tau^3\varepsilon(\partial_x^4 V)}^{\mathcal{O}(\varepsilon^4)}$$
$$+ \overbrace{\tfrac{1}{180}\tau^5\varepsilon(8\{(\partial_x^2 V)^2\partial_x^2 + \partial_x^2[(\partial_x^2 V)^2\cdot]\} - \{(\partial_x^3 V)(\partial_x V)\partial_x^2 + \partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot]}^{\mathcal{O}(\varepsilon^4)}$$
$$+ \overbrace{\tfrac{1}{90}\tau^5\varepsilon^{-3}\{(\partial_x^4 V)\partial_x^4 + \partial_x^4[(\partial_x^4 V)\cdot]\}}^{\mathcal{O}(\varepsilon^4)} + \mathcal{O}\left(\varepsilon^6\right)$$

and all odd powers of ε are gone!

We set $\mathcal{R}_1 = \frac{1}{2}\tau\varepsilon\partial_x^2$ and continue in this vein.

By the end of all this

$$
\begin{aligned}
\mathcal{R}_0 &= \tfrac{1}{2}\tau\varepsilon^{-1}V = \mathcal{O}(1),\\
\mathcal{R}_1 &= \tfrac{1}{2}\tau\varepsilon\partial_x^2 = \mathcal{O}(1),\\
\mathcal{R}_2 &= \tfrac{1}{24}\tau^3\varepsilon^{-1}(\partial_x V)^2 - \tfrac{1}{12}\tau^3\varepsilon\{(\partial_x^2 V)\partial_x^2 + \partial_x^2[(\partial_x^2 V)\cdot]\} = \mathcal{O}\left(\varepsilon^2\right),\\
\mathcal{R}_3 &= \tfrac{1}{120}\tau^5\varepsilon^{-1}(\partial_x^2 V)(\partial_x V)^2 + \tfrac{1}{24}\tau^3\varepsilon(\partial_x^4 V)\\
&\quad + \tfrac{1}{240}\tau^5\varepsilon\left(7\{(\partial_x^2 V)^2\partial_x^2 + \partial_x^2[(\partial_x^2 V)^2\cdot] + \{(\partial_x^3 V)(\partial_x V)\partial_x^2\right.\\
&\quad \left. + \partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot]\}\right) - \tfrac{1}{120}\tau^5\varepsilon^{-3}\{(\partial_x^4 V)\partial_x^4 + \partial_x^4[(\partial_x^4 V)\cdot]\}\\
&= \mathcal{O}\left(\varepsilon^4\right)
\end{aligned}
$$

and so on.

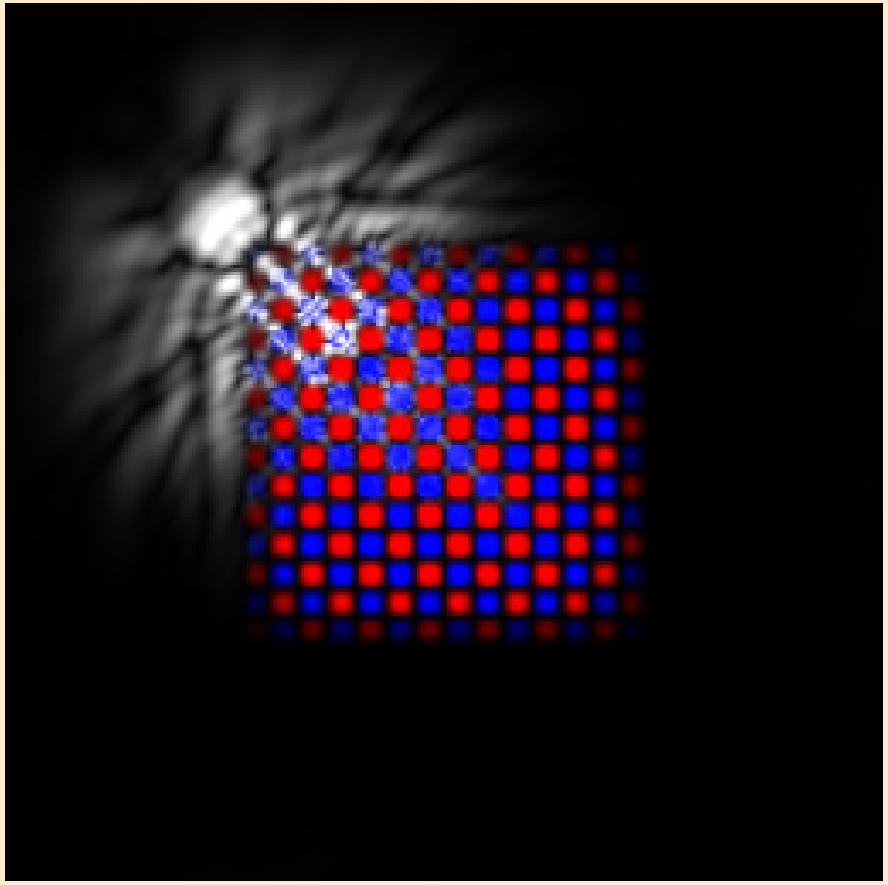
Note that U, ∂_x^{2k} symmetric $\Rightarrow$ $\mathrm{i}U, \mathrm{i}\partial_x^{2k}$ and $\mathrm{i}(U\partial_x^{2k} + \partial_x^{2k}U)$ are all skew-Hermitian, therefore each $\mathcal{R}_k$ is unitary. Therefore **the method is stable and preserves unitarity!!!**

Implementation: Now, and only now we discretise. We have used spectral collocation, therefore computing $\mathrm{e}^{\frac{1}{2}\tau\varepsilon^{-1}\mathcal{V}}\boldsymbol{v}$ and $\mathrm{e}^{\frac{1}{2}\tau\varepsilon\mathcal{D}}\boldsymbol{v}$ takes $\mathcal{O}(N)$and $\mathcal{O}(N\log N)$ (via FFT) operations respectively.

The vectors $\mathrm{e}^{\mathcal{R}_k}\boldsymbol{v}$ for $k\geq 2$ cannot be computed directly, but the $\mathcal{R}_k$ are *small:* $\mathcal{O}\left(\varepsilon^2\right)$ and $\mathcal{O}\left(\varepsilon^3\right)$. Therefore they can be computed to $\mathcal{O}\left(\varepsilon^6\right)$ using just three and two Krylov iterations resp.

While the analysis above was for $\sigma=1$, ideally we want $\sigma>0$ to be as small as possible, because this corresponds to large time steps. The entire approach works for $\sigma>\frac{1}{3}$ but probably the best compromise between large time steps and simple expressions is $\sigma=\frac{1}{2}$. In other words, $\Delta t\sim(\Delta x)^{1/2}$.

AN INTERMEZZO



Scattering of an electron off a square crystal lattice.

The method is a victim of its own success!!!

The reason for periodic boundary conditions is not physical: quantum particles (usually) don't live on a torus! The reason is that ***we can get away with it!***

Given that

1. Periodic boundary conditions allow us to use spectral methods or spectral collocation;
2. The solution is composed of wavepackets, hence highly localised: once we integrate it for a short time wavepackets never reach the boundary;

we can use periodic b.c.s without any ill effects.

But in our case point 2 does not apply! We can solve the equation with symmetric Zassenhaus for fairly long time intervals – and then we are in danger of false scattering off the boundary!

This motivates our interest in Dirichlet boundary conditions.

Part II: The joy and pain of skew symmetry

Although motivated by the

Semiclassical Schrödinger: $u_t = \mathrm{i}\varepsilon\Delta u + \mathrm{i}\varepsilon^{-1}V(\boldsymbol{x})u.$

we might just as well consider

The diffusion eqn: $u_t = \boldsymbol{\nabla}^\top a(\boldsymbol{x})\boldsymbol{\nabla}u, \qquad a > 0,$

Kinetic eqns: $u_t + \boldsymbol{V}(\boldsymbol{x})\cdot\boldsymbol{\nabla}u = B(u),$

Convection–diffusion: $u_t + \boldsymbol{V}(\boldsymbol{x})\cdot\boldsymbol{\nabla}u = \varepsilon\Delta u, \qquad \varepsilon > 0,$

Fokker–Planck: $u_t + \mathrm{div}[\mu(\boldsymbol{x})u] = B(\boldsymbol{x}, u).$

All involve coefficients that vary in space, hence standard methods of stability analysis don't apply: Fourier analysis because the coefficients vary and eigenvalue analysis since typically matrices aren't normal.

Except that a magic wand exists: Once space derivatives are discretised by a **skew symmetric matrix**, the method is stable!

A trivial (and misleading) example: 1D diffusion equation: Discretise $\partial_x u$ by $\mathcal{D}\boldsymbol{u}$ where $\mathcal{D} + \mathcal{D}^\top = O$. Then $\partial_x a(x)\partial_x$ is discretised by the negative definite matrix $\mathcal{D}\mathcal{A}\mathcal{D}$, where $\mathcal{A}$ is positive definite (since $a > 0$). This implies stability.

More importantly,

Theorem *(Al) Let*

1. The grid $\{x_m\}_{m=0}^{N+1}$ be dense in $[0, 1]$ for $N \gg 1$;
2. V be Lipschitz and $\mathcal{V}$ diagonal, $\mathcal{V}_{m,m} = V(x_m)$;
3. The differentiation matrix $\mathcal{D}$ be banded, skew-symmetric and such that $\max_{k,\ell} |\mathcal{D}_{k,\ell}| \leq b^\star N$ for some $b^\star > 0$.

Then both $\mathcal{V}\mathcal{D}$ and $\mathcal{D}\mathcal{V}$ are stable matrices: there exists $c > 0$ s.t.

$$\|\mathrm{e}^{t\mathcal{V}\mathcal{D}}\|, \|\mathrm{e}^{t\mathcal{D}\mathcal{V}}\| \leq 1 + ct.$$

The simplest is the best... The standard central-difference approximation

$$u'(x) = \frac{u(x+\Delta x) - u(x-\Delta x)}{2\Delta x}$$

on the uniform grid $x_m = \frac{m}{N+1}$ yields

$$\mathcal{D} = (N+1)\begin{bmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \cdots & 0 & -\frac{1}{2} & 0 \end{bmatrix},$$

a skew-symmetric matrix corresponding to a second-order discretisation.

This, however, is as far as we can go: as we will see soon, no third-order discretisation on a uniform grid can result in a skew-symmetric $\mathcal{D}$.

Conditions for skew symmetry (Ernst Hairer & Al): Let

$$0 = x_0 < x_1 < \cdots < x_N < x_{N+1} = 1$$

be a grid and $\mathcal{D}$ a differentiation matrix. Without loss of generality we can assume 0 b.c., hence p-order conditions are

$$\sum_{k=1}^{N} \mathcal{D}_{m,k} x_k^s (1 - x_k) = s x_m^{s-1} - (s+1) x_m^s, \qquad s = 1, \ldots, p-1.$$

Let

$$\varphi_s(x) = x^s (1-x)[(s+1) - (s+3)x], \qquad s \in \mathbb{N},$$
$$R^{[s]} = \sum_{k=1}^{N} \varphi_s(x_k).$$

Theorem *A necessary condition for a skew-symmetric matrix $\mathcal{D}$ to be of order $p \geq 2$ is*

$$R^{[1]} = R^{[2]} = \cdots = R^{[2p-3]} = 0.$$

Proof We note that the order conditions are

$$u'(x_m) = \sum_{k=1}^{N} \mathcal{D}_{m,k} u(x_k), \qquad m = 1, \ldots, N,$$

for every p-degree polynomial u that obeys zero b.c. Therefore, exploiting skew symmetry,

$$\sum_{m=1}^{N} u'(x_m) u(x_m) = \sum_{m=1}^{N} \sum_{k=1}^{N} u(x_m) \mathcal{D}_{m,k} u(x_k) = 0.$$

Letting $u(x) = x^s(1-x)$, $s = 1, \ldots, p-1$, we immediately have $\frac{1}{2} R^{[2s-1]} = 0$. Likewise, for $u(x) = x^s(1-x)^2$, $s = 1, \ldots, p-2$, we obtain $R^{[2s-1]} - 2R^{[2s]} + R^{[2s+1]} = 0$, therefore $R^{[2s]} = 0$. □

Theorem *If the grid is symmetric, $x_m + x_{N+1-m} \equiv 1$, then the order conditions reduce to $R^{[2s]} = 0$, $s = 1, \ldots, p-2$. In particular, such grid is always of order ≥ 2.*

For uniform grid $x_m = \frac{m}{N+1}$ we have $R^{[2]} = \frac{1}{6}\frac{N(N+2)}{(N+1)^3} \neq 0$ and order 3 is impossible!

To get order 3 with uniform grid we let even N and

$$x_m = \frac{\rho m}{N+1}, \quad x_{N+1-m} = 1 - x_m, \qquad m = 0, \ldots \lfloor N/2 \rfloor,$$

where ρ is a solution of the cubic

$$(3N^2 + 6N - 4)\rho^3 - 15N(N+2)\rho^2 + 24(N+1)^2\rho - 12(N+1)^2,$$

namely

$$\rho \sim 1 - \frac{8}{3}\frac{1}{N^2} + \frac{16}{3}\frac{1}{N^3} + \frac{128}{9}\frac{1}{N^4} - \frac{704}{9}\frac{1}{N^5} + \cdots.$$

Lemma *Let $\mathcal{D}$ be an $N \times N$, order-p differentiation matrix and suppose that $\mathcal{D}_{j,k} + \mathcal{D}_{k,j} = 0$ for all $1 \le \min\{j,k\} \le N-p-1$. Then $\mathcal{D}$ is skew symmetric.*

Proof Let $u(x) = x(1-x)\tilde{u}(x)$, where $\deg \tilde{u} \le p-2$. Because of the above condition,

$$0 = \sum_{m=1}^{N} u(x_m)u'(x_m) = \sum_{m=1}^{N}\sum_{k=1}^{N} u(x_m)\mathcal{D}_{m,k}u(x_k) = \sum_{m=N-p+2}^{N}\sum_{k=N-p+2}^{N} u(x_m)\mathcal{D}_{m,k}u(x_k).$$

Choose $s \in \{N-p+2, \ldots, N\}$ and set $\tilde{u} = \ell_s$, where

$$\ell_s(x) = \prod_{\substack{j=N-p+2 \\ j\neq s}}^{N} \frac{x - x_j}{x_s - x_j}.$$

Then

$$0 = \sum_{m=N-p+2}^{N}\sum_{k=N-p+2}^{N} u(x_m)\mathcal{D}_{m,k}u(x_k) = x_s^2(1-x_s)^2\mathcal{D}_{s,s}$$

and we conclude that $\mathcal{D}_{k,k} = 0$, $k = 1, \ldots, N$. Next, choose $\tilde{u} = \ell_q + \ell_s$ for distinct q, s in $\{N-p+2, \ldots, N\}$. Then

$$0 = \sum_{m=N-p+2}^{N}\sum_{k=N-p+2}^{N} u(x_m)\mathcal{D}_{m,k}u(x_k) = x_q(1-x_q)x_s(1-x_s)(\mathcal{D}_{q,s} + \mathcal{D}_{s,q})$$

and the proof of skew symmetry is complete. □

Theorem *The condition*

$$R^{[1]} = R^{[2]} = \cdots = R^{[2p-3]} = 0$$

is sufficient for skew-symmetry of $\mathcal{D}$*.*

Proof By construction. We need to construct the leading $N - p - 1$ rows and columns of $\mathcal{D}$ and assume that the grid obeys the above condition. Commence from the top row, setting $\mathcal{D}_{1,1} = 0$. We have $N - 1$ remaining parameters and $p - 1$ order conditions: fix $N - p$ entries and solve a (nonsingular) Vandermonde linear system for the remaining ones. Extend to the first column by skew symmetry.

We continue in this vain to the second row etc., until the $(N - p - 1)$st row, always having $\geq p - 1$ parameters. This, combined with the previous theorem, concludes the proof. □

Corollary *Subject to above conditions there exists a* $(2p + 1)$*-diagonal skew-symmetric differentiation matrix of order* p*.*

Size (sometimes) matters Our original setting required that $|\mathcal{D}_{k,\ell}| \leq b^\star N$ uniformly for all k, ℓ and $n \gg 1$. Does this hold for the banded matrices from the corollary?

Sometimes it does and all is well,
Sometimes it doesn't but, nonetheless, all is well, and
Sometimes it doesn't and things go haywire.

It is at present unclear for which grids the increase is uniformly linear. Moreover, even if the condition fails, the approximation is stable for *some* potentials V. A clue to this discrepancy might be this: In the theorem we need to bound $\|\mathrm{e}^{t\mathcal{V}\mathcal{D}}\|$, but instead we bound its upper bound, $\mathrm{e}^{t\alpha[\mathcal{V}\mathcal{D}]}$, where $\alpha[A] = \max\sigma(\frac{1}{2}(A + A^\top))$ is the logarithmic norm of A.

Grid is (occasionally) good It is possible, for any $p \geq 2$, to find a grid consistent with order p and skew symmetry (Kai Lau). However, we want much more!

Typically, a grid is determined by an adaptive algorithm in response to local behaviour of the solution, e.g. boundary and internal layers. Our objective is to commence from a *given* grid and perturb it mildly to satisfy order conditions. Is this possible?

We commence from a strictly monotone grid function g s.t. $g(0) = 0$, $g(1) = 1$, and let $\tilde{x}_m = g(m/(N+1))$, $m = 1, \ldots, N$. The objective is to find a perturbed grid $x_m = \tilde{x}_m + \mathcal{O}\left(N^{-2}\right)$, $m = 1, \ldots, N$, that obeys order-p and skew-symmetry conditions.

Lemma *Let*

$$I_s[g] = \int_0^1 g^s(\tau)[1 - g(\tau)][(s+1) - (s+3)g(\tau)]\,\mathrm{d}\tau, \qquad s \in \mathbb{N}.$$

A necessary condition for the existence of a perturbed grid is $I_s[g] = 0$ *for* $s = 1, \ldots, 2p-3$.

Lemma *The equalities of the last lemma hold iff the inverse function* g^{-1} *is orthogonal to shifted Legendre polynomials* $\tilde{\mathsf{P}}_m$, $m = 2, \ldots, s+1$.

Theorem *If* $I_1[g] = 0$ *then there exists a perturbed grid consistent with 2nd-order conditions.*

The proof of the last theorem is constructive.

Negative-definite approximation of the Laplace–Beltrami operator

Once $\mathcal{D}$ is a skew-symmetric differentiation matrix, while $\mathcal{A}$ is positive definite, $\mathcal{D}_2 = \mathcal{D}\mathcal{A}\mathcal{D}$, an approximation of $\partial_x[a(x)\partial_x]$, is nonpositive definite. The bad news is though that $\mathcal{D}_2$ has plenty of zero entries that generate spurious oscillations in $\mathrm{e}^{t\mathcal{D}_2}$.

Instead, we use staggered grids

$$0 = x_0 < y_0 < x_1 < y_1 < \cdots < y_{N-1} < x_N < y_N < x_{N+1} = 1.$$

Specifically,

$$u'(x_m) \approx \sum_{\ell=0}^{N+1} \mathcal{D}_{m,\ell} u(y_\ell), \qquad u'(y_\ell) \approx \sum_{m=1}^{N} \mathcal{E}_{\ell,m} u(x_m).$$

It is trivial to prove that $\mathcal{E}^\top = -\mathcal{D}$ implies that $\mathcal{E}\mathcal{A}\mathcal{D}$ is nonpositive definite.

The research here is incomplete, yet promising.

Part III: Into the unknown– spectral methods

Spectral methods: Expansion in a rapidly-convergent basis $\{\varphi_n\}_{n\in\mathbb{Z}_+}$.

Periodic b.c.: Fourier basis, $\varphi_{2n}(x) = \mathrm{e}^{\mathrm{i}\pi n\theta}$, $\varphi_{2n+1}(x) = \mathrm{e}^{-\mathrm{i}\pi n\theta}$, convergence in $\mathrm{C}^\infty[0,1]$ at spectral speed (faster than the reciprocal of any polynomial). Moreover, the differentiation matrix is skew Hermitian.

Dirichlet b.c.: Typically, a polynomial basis (Chebyshev or Legendre). Hence

$$\varphi_n' \in \mathrm{Span}\,\{\varphi_0, \ldots, \varphi_{n-1}\}$$

and the differentiation matrix can't be skew symmetric.

Initial thoughts on a possible avenue of attack...

The idea: start from a skew-symmetric matrix and *construct* a basis. E.g., consider a tridiagonal symmetric matrix and seek a vector function φ s.t.

$$\varphi' = \begin{bmatrix} 0 & b_0 & 0 & \cdots \\ -b_0 & 0 & b_1 & \ddots \\ 0 & -b_1 & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{bmatrix} \varphi,$$

where $b_n \neq 0$. In other words,

$$\varphi_0' = b_0\varphi_1, \qquad \varphi_n' = -b_{n-1}\varphi_{n-1} + b_n\varphi_{n+1}, \quad n \in \mathbb{N}.$$

The trick is to fix $\varphi_0 \in \mathsf{C}^\infty$, whereby

$$\varphi_n = \frac{1}{b_n}(b_{n-1}\varphi_{n-1} + \varphi_n') \;\Rightarrow\; \phi_n = \frac{1}{b_0 b_1 \cdots b_{n-1}} \sum_{\ell=0}^{\lfloor n/2 \rfloor} \alpha_{n,\ell}\varphi_0^{(n-2\ell)}$$

for some $\alpha_{n,\ell}$s.

An example: $b_0 = \sqrt{2}/2$, $b_n = -1/2$, $n \in \mathbb{N}$ and $\varphi_0(x) = \mathsf{J}_0(x)$ yields $\varphi_n(x) = (-1)^{n+1}\sqrt{2}\mathsf{J}_n(x)$, $n \in \mathbb{N}$. Here J_n is a Bessel function.

Another example: Let $b_n \equiv 1$ and $\varphi_0(x) = \mathrm{e}^{-x^2}$. Then

$$\varphi_{2n} = \mathrm{e}^{-x^2} \sum_{m=0}^{n} \binom{n+m}{2m} \mathrm{H}_{2m},$$

$$\varphi_{2n+1} = -\mathrm{e}^{-x^2} \sum_{m=0}^{n} \binom{n+m+1}{2m+1} \mathrm{H}_{2m+1},$$

where H_n is the Hermite polynomial.

The desiderata:

1. $\{\varphi_n\}_{n\in\mathbb{Z}_+}$ is an orthogonal system spanning $\mathrm{L}[0,1]$;
2. An expansion in φ_ns converges spectrally fast in $\mathrm{C}^\infty[0,1]$;
3. The expansion coefficients can be computed by a fast algorithm.

The above examples all fail on each of these points.

A *very* recent development (Helge Dietert, Al & Caroline Lasser): Let

$$\varphi_n(x) = \frac{(-1)^n}{\sqrt{2^n n!}} \mathrm{e}^{-\frac{1}{2}x^2} \mathsf{H}_n(x), \qquad n \in \mathbb{Z}_+.$$

We have

$$\varphi_n'(x) = -b_{n-1}\varphi_{n-1}(x) + b_n \varphi_{n+1}(x), \quad n \in \mathbb{Z}_+,$$

where $b_n = \sqrt{(n+1)/2}$. Moreover,

$$\pi^{-1/2} \int_{-\infty}^{\infty} \varphi_m(x)\varphi_n(x)\,\mathrm{d}x = \delta_{m,n}, \qquad m, n \in \mathbb{Z}_+.$$

Under obvious transformation, we are dealing with Hermite-type expansion:

$$f(x) = \mathrm{e}^{-\frac{1}{2}x^2} \sum_{n=0}^{\infty} \widehat{f}_n \mathsf{H}_n(x), \qquad \widehat{f}_n = \frac{1}{2^n n!} \int_{-\infty}^{\infty} f(x) \mathsf{H}_n(x) \mathrm{e}^{-\frac{1}{2}x^2}\,\mathrm{d}x,$$

which is orthogonal and converges spectrally fast. But can the coefficients be computed fast?

Another recent development (Helge Dietert, Al & Caroline Lasser)
(a variation on ideas of **Daan Huybrechs & Haiyong Wang**): How to buy a hat with a check?
An algorithm to compute

$$\hat{f}_0, \ldots, \hat{f}_{N-1}, \qquad \text{where} \qquad f(x) = \sum_{n=0}^{\infty} \hat{f}_n \mathsf{H}_n(x),$$

to an arbitrary accuracy in $\mathcal{O}(N \log_2 N)$ operations.

1. Let $s = s_N \gg 1$. Compute interpolation to f at the *stretched Chebyshev points* $s \cos \frac{k-\frac{1}{2}}{N}$, $k = 1, \ldots, N$. This can be done with a single FFT and yields

$$f(x) \approx \check{f}(x) = \sum_{n=0}^{N-1} \check{f}_n \mathsf{T}_n(sx).$$

Note that $|\check{f}(x) - f(x)|$ is spectrally small for $f \in \mathsf{C}(\mathbb{R})$ and $x \in \mathbb{R}$.

2. Convert the $\check{f}_m$s to $\widehat{f}_n$ by computing the *Chebyshev-to-Hermite connection coefficients*

$$\rho_{m,n} = \pi^{-1/2} \int_{-\infty}^{\infty} \mathsf{T}_m(sx)\mathsf{H}_n(x)\mathrm{e}^{-x^2/2}\,\mathrm{d}x, \qquad m,n \in \mathbb{Z}_+.$$

Then

$$\widehat{f}_n = \frac{1}{2^n n!} \sum_{m=n}^{N-1} \check{f}_m \rho_{m,n}, \qquad n = 0,\ldots,N-1.$$

3. Unfortunately, computing $\rho_{m,n}$ for $0 \le m \le n \le N-1$ and then computing the $\widehat{f}_n$ takes $\mathcal{O}\left(N^2\right)$ operations. Instead, truncate the expression: Let $q \ge 1$ be an integer and set

$$\widehat{f}_n^{[q]} = \frac{1}{2^n n!} \sum_{m=n}^{\min\{n+q,N-1\}} \check{f}_m \rho_{m,n}, \qquad n = 0,\ldots,N-1.$$

If s_N and q are large enough then $|\widehat{f}_n^{[q]} - \widehat{f}_n|$ is spectrally small and we are done in $\mathcal{O}(N \log_2 N)$ operations!

Final comments

★ Stability and unitarity are best achieved by skew-symmetric differentiation matrices. They are easy to construct (whether with finite differences or spectral methods) for periodic boundary conditions but...

★ The construction of skew-symmetric differentiation matrices with Dirichlet b.c.s is difficult. For finite differences it requires the construction of 'exotic' grids and high orders might be beyond reach, while for spectral methods just one, fresh off the press, approach is available.

★ This analysis applies to a wide range of linear PDEs of evolution with variable coefficients, e.g. semiclassical Schrödinger, Liouville and convection–diffusion. But it is also relevant to nonlinear PDEs via operatorial splittings, e.g. to kinetic equations (Boltzmann, Vlasov–Poisson, ...).

So, what is *really* FoCM?