Symplectic methods for the time integration of the Schrödinger equation

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Joint work with:
Fernando Casas and Ander Murua

The Goal

The numerical integration of the time-dependent Schrödinger Equationt ($\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2\mu}\nabla^2\psi(x,t) + V(x)\psi(x,t)$$

$\psi(x,0) = \psi_0(x),\ x \in \mathbb{R}^D,\ t \in [0, T].$

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We consider the case where an appropriate spatial discretisation is used and one has to solve an IVP

The Numerical Integration of Differential Equations

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About 50 years ago, researchers had the hope to develop a few numerical methods to cover the numerical solution of most problems, i.e. to build a black box with a few number of methods implemented.
Soon, it was clear that this was too optimistic due to the huge variety of problems of very different nature, and started to look for methods tailored for different classes of problems

Different families of methods

- Runge–Kutta methods (explicit and implicit)
- Multistep methods (explicit and implicit)
- Extrapolation methods
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However, most equations to be solved originate from physical problems obtained from First Principles, which makes the solutions to have very particular qualitative properties.
Geometric Integration

- Symplectic Integrators
- Lie group methods
- Volume-preserving methods
- etc.

The numerical Solution of very particular problems

The development of computers allowed to researchers in physics, chemistry, engineering, etc. to study more challenging problems from the computational point of view.

These problems can not be solved by the computer just by brute force, and tailored methods have to be developed.

Example

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- for 60 Myrs
- Backward in time
- to very high accuracy

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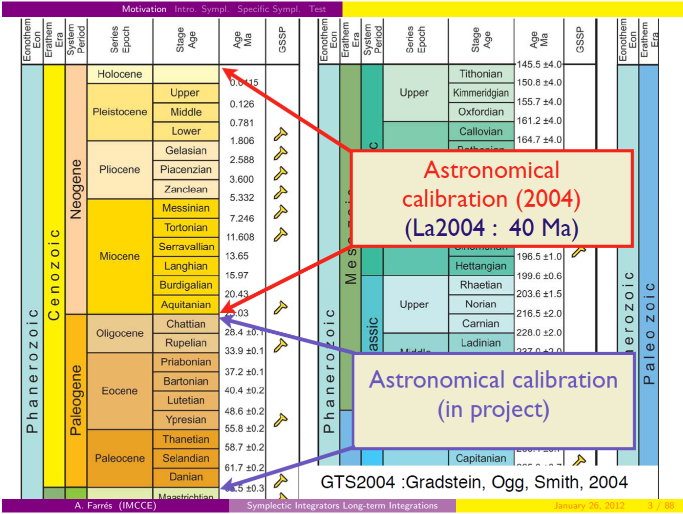
This problem comes from a research collaboration between geologists and astronomers.
Actual methods (already tailored for this problem) allowed for a faithful integration over 40 Myrs, with good agreement with observations by geologists.
We were asked to develop new methods with better performance than the existing ones for this particular problem.

Example:



B, Casas, Farrés, Makazaga, Murua and Laskar. Two submitted papers.

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- Numerical Methods valid for most problems
- Numerical methods useful for a class of problems
- Numerical methods tailored for one problem

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We present with some detail the steps to follow in order to look for efficient methods for some problems in Quantum Mechanics.

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4. (Practical) To collaborate with experts on these fields

Back to the Physical Problem

We illustrate this procedure on the 1-dim SE

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = \mathcal{H}\psi(x,t)$$

$\psi(x,0) = \psi_0(x)$. $\mathcal{H}$ is an Hermitian operator.

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$\psi(x,0) = \psi_0(x)$. $\mathcal{H}$ is an Hermitian operator. Then

$$\mathcal{H}\varphi_k(x) = \mathcal{E}_k\varphi_k(x), \qquad k = 0, 1, 2, \ldots$$

where $\{\mathcal{E}_k, \varphi_k(x)\}$ are the real eigenvalues and orthonormal eigenfunctions, and

$$\psi_0(x) = \sum_{k=0}^{\infty} c_k\varphi_k(x) \qquad \Rightarrow \qquad \psi(x,t) = \sum_{k=0}^{\infty} c_k e^{-it\mathcal{E}_k}\varphi_k(x)$$

Back to the problem

- $|\psi(x,t)|^2$: probability to find the quantum particle in (x,t)
- Then, $\psi(x,t) \to 0$ as $x \to \pm\infty$
- It suffices to consider a bounded region where the solution and all its derivatives vanishes at the boundaries (periodic problem)
- We can use spectral methods for the spatial discretisation

Back to the problem

A mesh with d points $\Rightarrow$ d-dimensional linear problem

$$i\,\frac{d}{dt}u = H\,u \quad \Rightarrow \quad u(T) = e^{-i\,T\,H}u(0)$$

where $u \in \mathbb{C}^d$ and $H \in \mathbb{R}^{d\times d}$ is a Hermitian matrix.

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$$H v_k = E_k v_k, \qquad k = 0, 1, 2, \ldots, d-1$$

where we expect

$$E_k \simeq \mathcal{E}_k, \qquad v_{k,j} \simeq \psi_k(x_j)$$

for $k = 0, 1, \ldots, d_0 - 1$ with $d_0 \leq d$, and

$$u_0 = \sum_{k=0}^{d-1} \hat{c}_k v_k, \qquad \Rightarrow \qquad u(T) = \sum_{k=0}^{d-1} \hat{c}_k e^{-i\,T\,E_k} v_k$$

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Formally, the problem to solve is

$$i\frac{du}{dt} = P^{-1} \begin{pmatrix} E_0 & & & \\ & E_1 & & \\ & & \ddots & \\ & & & E_{d-1} \end{pmatrix} Pu = Hu$$

which is just a set of d harmonic oscillators

The goal: To approximate the solution

$$u(T) = e^{-i\,T\,H}\,u_0$$

using an algorithm which involves vector-matrix products.
Inputs:

- T: Time of integration.
- u_0: Initial conditions.
- Hu: A subroutine, to compute the product of a vector u with the matrix H.
- E_{min}, E_{max}, such that

  $$E_{min} \le E_0 < \ldots < E_{d-1} \le E_{max}$$

  (they are usually known).
- tol: The approximated solution, $\tilde{u}$, must satisfy

  $$\|u(T) - \tilde{u}\| < tol$$

We can take a shift to the center of the eigenvalues

$$e^{-itH} = e^{-i\,T\,\alpha} e^{-i\,T\,(H - \alpha I)}$$

with

$$\alpha = \frac{E_{\mathrm{max}} + E_{\mathrm{min}}}{2}$$

and a normalization

$$\exp\left(-iTH\right) = \exp\left(-i\,T\,\alpha\right)\ \exp\left(-i\,T\,\beta\tilde{H}\right)$$

where

$$\tilde{H} = \frac{H - \alpha I}{\beta}, \qquad \beta = \frac{E_{\mathrm{max}} - E_{\mathrm{min}}}{2}$$

so

$$-1 \leq \sigma(\tilde{H}) \leq 1$$

The Mathematical Problem

To approximate

$$w(T) = e^{-i\,T\,\beta\,\tilde{H}} u_0$$

where

$$\beta = \frac{E_{\max} - E_{\min}}{2}, \qquad -1 \leq \sigma(\tilde{H}) \leq 1$$

$$\tau = T\beta \qquad (\textit{effective time})$$

using polynomial approximations (vector matrix products) such that

$$\|w(T) - w_{ap}\| < tol$$

The State of the Art: Taylor method

$(u = q + ip)$

$$w_T = \sum_{k=0}^{m} \frac{(-i\,T\,\beta)^k}{k!} \tilde{H}^k u_0 = (T_m^C - iT_m^S)(q_0 + ip_0)$$

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Horner's algorithm

$$\begin{array}{l} y_0 = u_0 \\ \textbf{do} \;\; k = 1, m \\ \quad y_k = u_0 - i\frac{T\beta}{m+1-k}\tilde{H}y_{k-1} \\ \textbf{enddo} \\ w_T = y_m \end{array}$$

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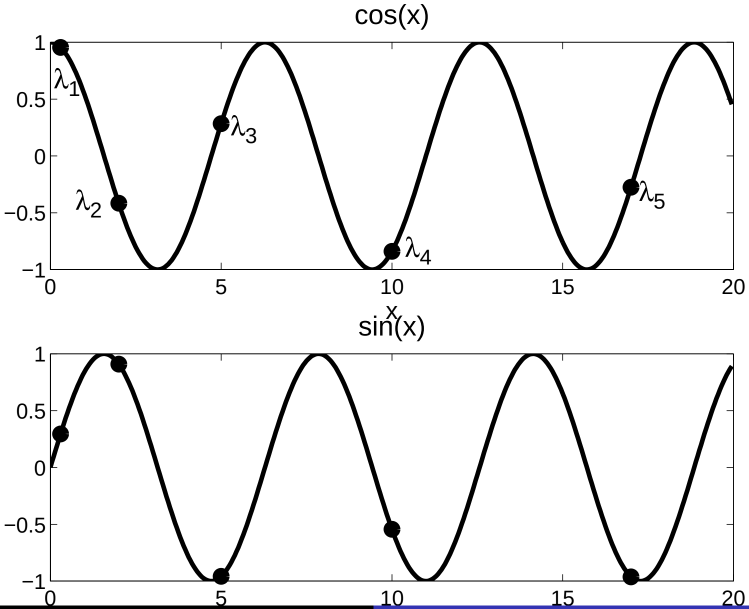
Error bounds

$$\|w(T) - w_T\| < \frac{(T\beta)^{m+1}}{(m+1)!} e^{T\beta}, \qquad \frac{T\,\beta}{m} \lesssim 0.3$$

Example:



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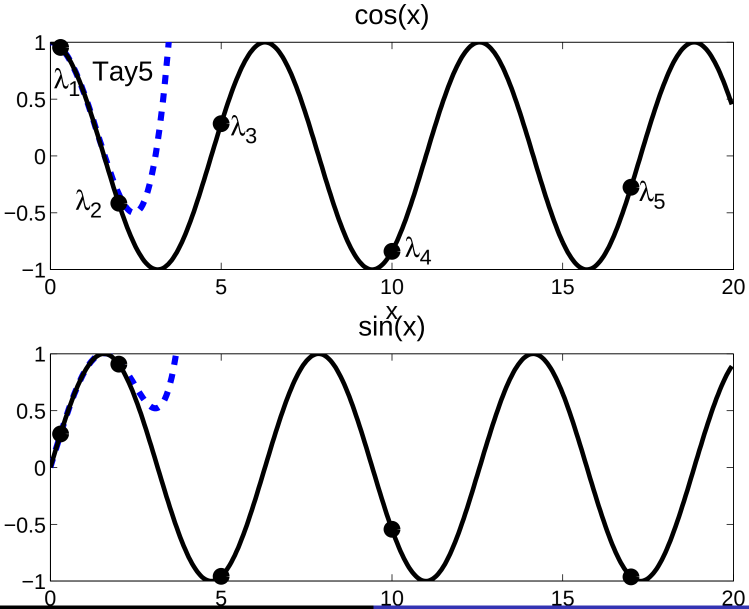
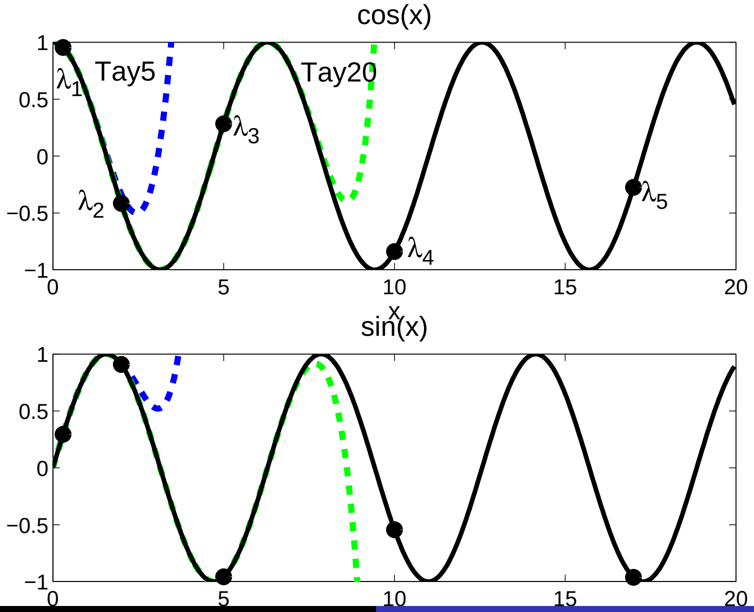


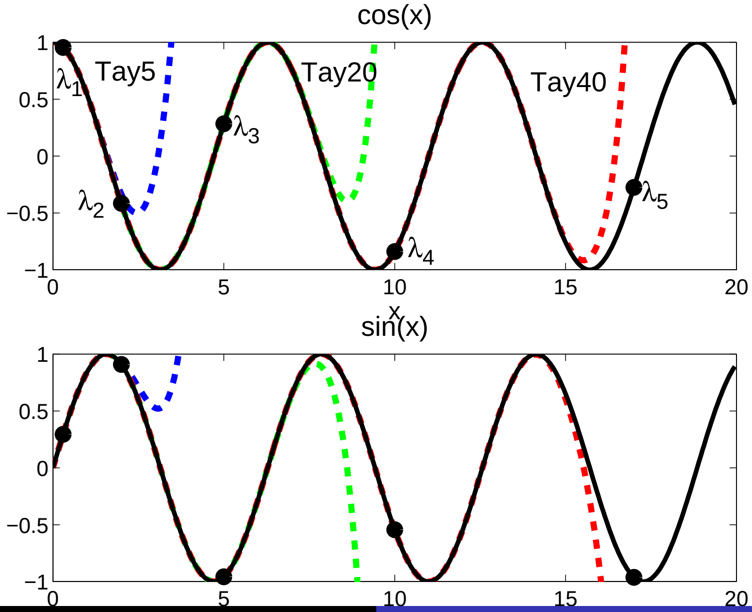
cos(x)
Tay5
λ1
λ2
λ3
λ4
λ5
1
0.5
0
−0.5
−1
0
5
10
15
20
x
sin(x)
1
0.5
0
−0.5
−1
0
5
10
15
20

Example:

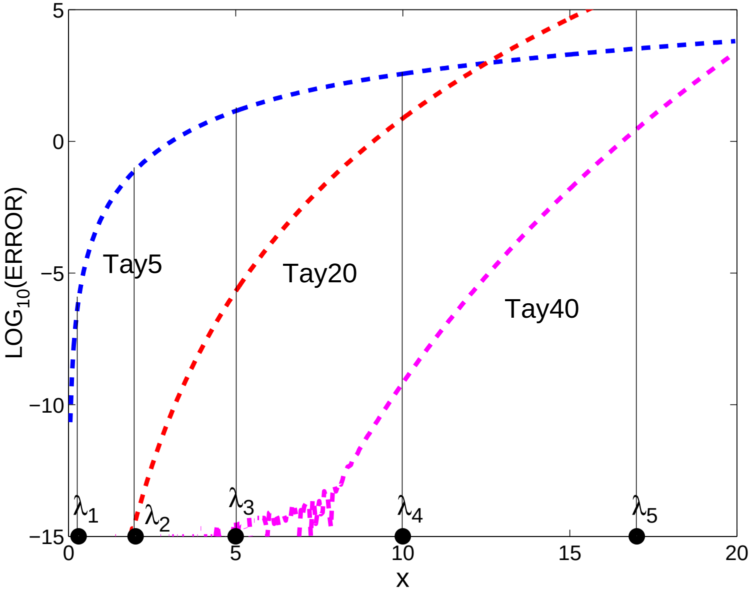


cos(x)
1
0.5
0
−0.5
−1
0
5
10
15
20
x
Tay5
Tay20
λ1
λ2
λ3
λ4
λ5
sin(x)
1
0.5
0
−0.5
−1
0
5
10
15
20

Example:


cos(x)
Tay5
Tay20
Tay40
λ_1
λ_2
λ_3
λ_4
λ_5
x
sin(x)

Example:



5
0
−5
−10
−15
0
5
10
15
20
x
LOG_{10}(ERROR)
Tay5
Tay20
Tay40
λ_1
λ_2
λ_3
λ_4
λ_5

The State of the Art: Chebyshev method

$$w_C = \left(J_k(T\beta) + 2\sum_{k=1}^{m} (-i)^k J_k(T\beta)\, T_k(\tilde{H}) \right) u_0 = (C_m^C - iC_m^S)(q_0 + ip_0)$$

$J_k(t)$: Bessel functions of the first kind
$T_k(x)$: kth Chebyshev polynomial

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The Clenshaw algorithm ($c_k = (-i)^k J_k(\tau\,\beta)$):

$$d_{m+2} = 0, \qquad d_{m+1} = 0$$

do $k = m, 0$

$$d_k = c_k u_0 + 2\tilde{H} d_{k+1} - d_{k+2}$$

enddo

$$w_C \equiv P_{m-1}^C(\tau \tilde{H})\, u_0 = d_0 - d_2$$

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&\textbf{do}\;\; k = m, 0 \\
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&\textbf{enddo} \\
&w_C \equiv P_{m-1}^C(\tau \tilde{H})\, u_0 = d_0 - d_2
\end{aligned}$$

Error bounds

$$\|w(T) - w_C\| < 4 \left(\mathrm{e}^{1-(\beta\tau/2(m+1))^2} \frac{\beta\tau}{2(m+1)} \right)^{(m+1)}, \qquad \frac{T\,\beta}{m} < 1$$

The State of the Art: Symplectic methods

$$u = e^{-iT\beta\tilde{H}}u_0 \quad \Rightarrow \quad q + ip = (\cos(T\beta\tilde{H}) - i\sin(T\beta\tilde{H}))(q_0 + ip_0)$$

$$\left\{ \begin{array}{c} q \\ p \end{array} \right\} = \left(\begin{array}{cc} \cos(T\beta\tilde{H}) & \sin(T\beta\tilde{H}) \\ -\sin(T\beta\tilde{H}) & \cos(T\beta\tilde{H}) \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\}$$

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$$\begin{Bmatrix} q \\ p \end{Bmatrix} = \begin{pmatrix} \cos(T\beta\tilde{H}) & \sin(T\beta\tilde{H}) \\ -\sin(T\beta\tilde{H}) & \cos(T\beta\tilde{H}) \end{pmatrix} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix}$$

Splitting Symplectic methods

$$\begin{Bmatrix} q_S \\ p_S \end{Bmatrix} = \prod_{k=1}^{m} \begin{pmatrix} I & 0 \\ -b_k T\beta\tilde{H} & I \end{pmatrix} \begin{pmatrix} I & a_k T\beta\tilde{H} \\ 0 & I \end{pmatrix} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix}$$

Gray & Manolopoulos J. Chem. Phys. (1996): $m = 2, 4, 6, 8, 10, 12$

The algorithm:

$$\begin{aligned} &\textbf{do} \ \ k = 1, m \\ &\quad q := q + a_k T\beta\tilde{H}p \\ &\quad p := p - b_k T\beta\tilde{H}q \\ &\textbf{enddo} \end{aligned} \qquad \frac{T\beta}{m} < 2$$

NO Error bounds

Numerical example 1

(Lubich, Blue book, 2008) To approximate

$$e^{-iH}u_0$$

with u_0 a unitary random vector and

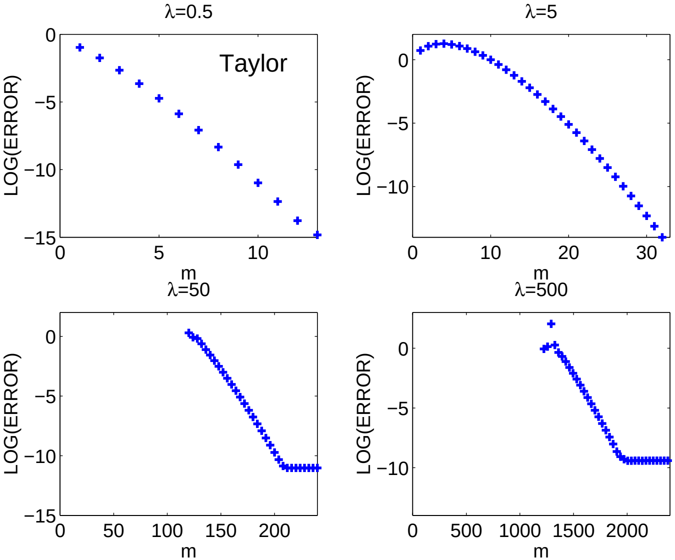
$$H = \frac{\lambda}{2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{N\times N}, \quad N = 10000$$

$0 \le E_k \le 2\lambda,\; k = 1, 2, \ldots, 10000$
After a shift, $H - \lambda I$, we can take: $T\beta = \lambda$
We approximate:

$$e^{-i\lambda}e^{-i\lambda\hat{H}}u_0, \qquad \hat{H} = (H - \lambda I)/\lambda$$

$$\lambda = 0.5, \quad \lambda = 5, \quad \lambda = 50, \quad \lambda = 500$$

Example 1:


λ=0.5
Taylor
LOG(ERROR)
0
−5
−10
−15
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5
10
m
λ=5
LOG(ERROR)
0
−5
−10
0
10
20
30
m
λ=50
LOG(ERROR)
0
−5
−10
−15
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50
100
150
200
m
λ=500
LOG(ERROR)
0
−5
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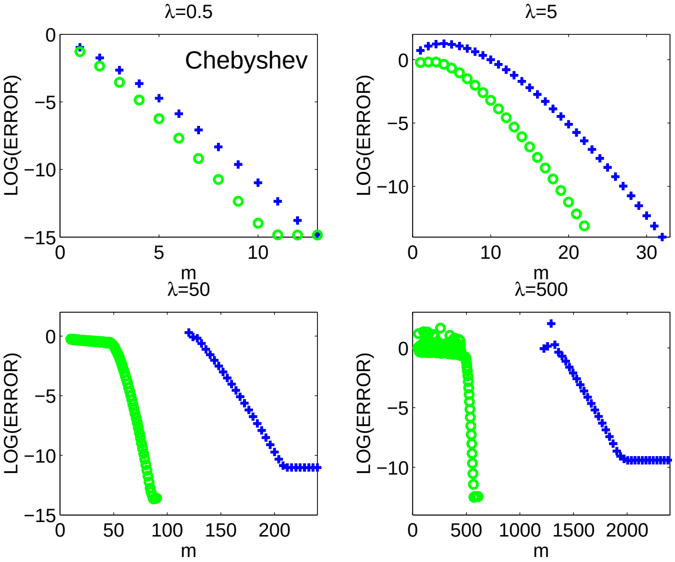
500
1000
1500
2000
m

Example 1:


λ=0.5
Chebyshev
LOG(ERROR)
m
λ=5
LOG(ERROR)
m
λ=50
LOG(ERROR)
m
λ=500
LOG(ERROR)
m

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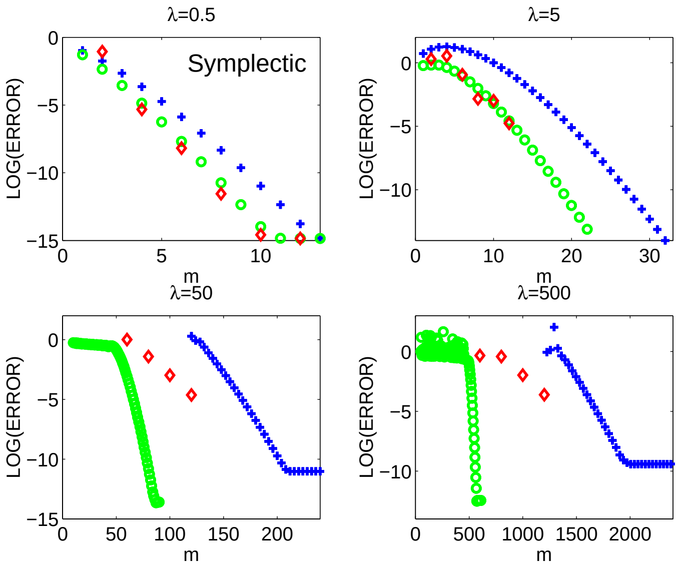

λ=0.5
Symplectic
LOG(ERROR)
m
0
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−10
−15
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5
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λ=5
LOG(ERROR)
m
0
−5
−10
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10
20
30
λ=50
LOG(ERROR)
m
0
−5
−10
−15
0
50
100
150
200
λ=500
LOG(ERROR)
m
0
−5
−10
0
500
1000
1500
2000

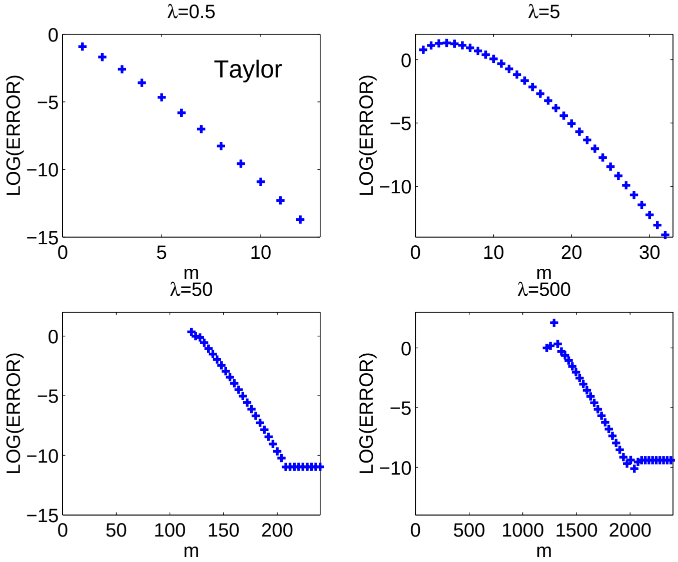
Numerical example 2: The scalar problem

$$e^{-i\lambda}u_0, \qquad \lambda \in \mathbb{R}$$

with $u_0 = 1$

$$\lambda = 0.5, \quad \lambda = 5, \quad \lambda = 50, \quad \lambda = 500$$

Example 2:



λ=0.5
Taylor
LOG(ERROR)
0
−5
−10
−15
0
5
10
m
λ=5
LOG(ERROR)
0
−5
−10
0
10
20
30
m
λ=50
LOG(ERROR)
0
−5
−10
−15
0
50
100
150
200
m
λ=500
LOG(ERROR)
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−5
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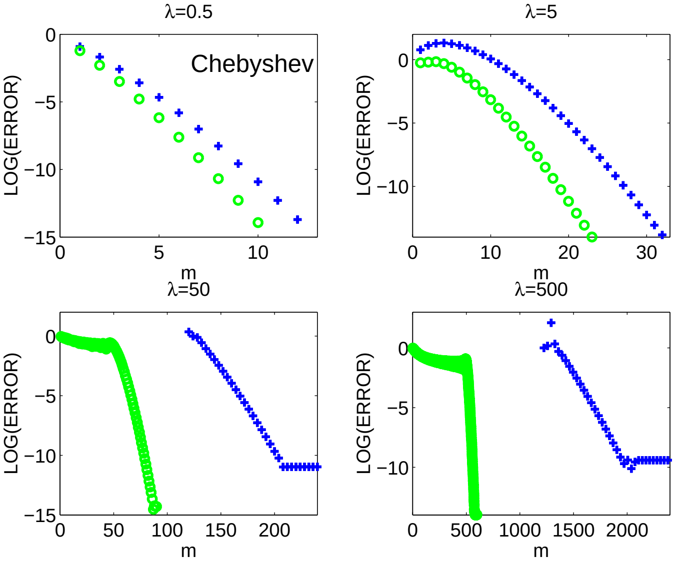
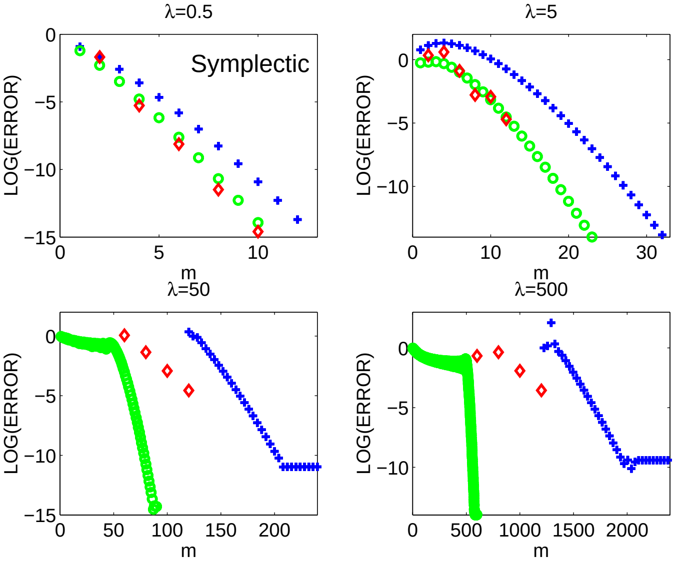
0
500
1000
1500
2000
m

Example 2:


λ=0.5
Chebyshev
LOG(ERROR)
m
λ=5
LOG(ERROR)
m
λ=50
LOG(ERROR)
m
λ=500
LOG(ERROR)
m

Example 2:


λ=0.5
Symplectic
LOG(ERROR)
m
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LOG(ERROR)
m
λ=50
LOG(ERROR)
m
λ=500
LOG(ERROR)
m

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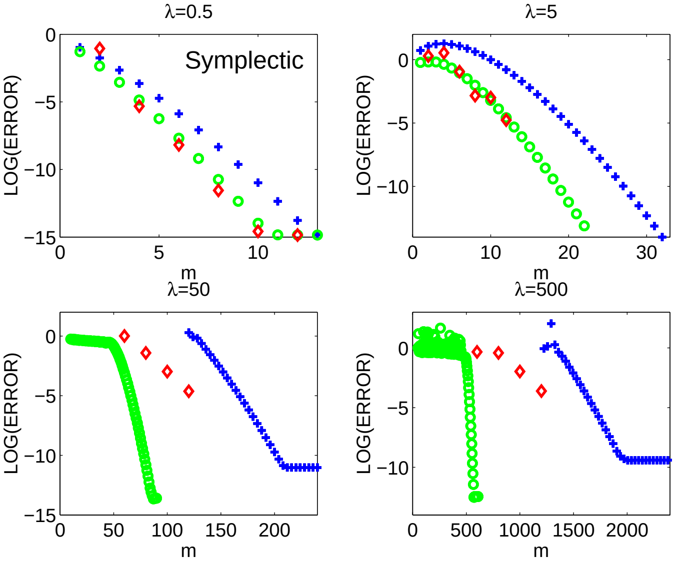

λ=0.5
Symplectic
LOG(ERROR)
m
λ=5
LOG(ERROR)
m
λ=50
LOG(ERROR)
m
λ=500
LOG(ERROR)
m

The Simplified Model

$$u = e^{-iy} u_0 \quad \Rightarrow \quad q + ip = (\cos(y) - i\sin(y))(q_0 + ip_0)$$

$$\left\{ \begin{array}{c} q \\ p \end{array} \right\} = \left(\begin{array}{cc} \cos(y) & \sin(y) \\ -\sin(y) & \cos(y) \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\}$$

Taylor method

$$\left\{ \begin{array}{c} q_T \\ p_T \end{array} \right\} = \left(\begin{array}{cc} T_1^m & T_2^m \\ -T_2^m & T_1^m \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\}$$

$$\frac{T\,\beta}{m} < 0.3$$

Taylor method

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$$\frac{T\,\beta}{m} < 0.3$$

Chebyshev method

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$$\frac{T\,\beta}{m} < 1$$

Taylor method

$$\left\{ \begin{array}{c} q_T \\ p_T \end{array} \right\} = \left(\begin{array}{cc} T_1^m & T_2^m \\ -T_2^m & T_1^m \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} \qquad \frac{T\,\beta}{m} < 0.3$$

Chebyshev method

$$\left\{ \begin{array}{c} q_C \\ p_C \end{array} \right\} = \left(\begin{array}{cc} C_1^m & C_2^m \\ -C_2^m & C_1^m \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} \qquad \frac{T\,\beta}{m} < 1$$

Symplectic methods

$$\left(\begin{array}{cc} 1 & 0 \\ -b_k y & 1 \end{array} \right) \left(\begin{array}{cc} 1 & a_k y \\ 0 & 1 \end{array} \right) = \left(\begin{array}{cc} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{array} \right)$$

Taylor method

$$\begin{Bmatrix} q_T \\ p_T \end{Bmatrix} = \begin{pmatrix} T_1^m & T_2^m \\ -T_2^m & T_1^m \end{pmatrix} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix} \qquad \frac{T\beta}{m} < 0.3$$

Chebyshev method

$$\begin{Bmatrix} q_C \\ p_C \end{Bmatrix} = \begin{pmatrix} C_1^m & C_2^m \\ -C_2^m & C_1^m \end{pmatrix} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix} \qquad \frac{T\beta}{m} < 1$$

Symplectic methods

$$\begin{pmatrix} 1 & 0 \\ -b_k y & 1 \end{pmatrix} \begin{pmatrix} 1 & a_k y \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{pmatrix}$$

$$K(y) \equiv \prod_{k=1}^{m} \begin{pmatrix} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{pmatrix} = \begin{pmatrix} K_1^{2m-2} & K_2^{2m-1} \\ K_3^{2m-1} & K_4^{2m} \end{pmatrix}$$

$$\begin{Bmatrix} q_S \\ p_S \end{Bmatrix} = \begin{pmatrix} K_1^{2m-2} & K_2^{2m-1} \\ K_3^{2m-1} & K_4^{2m} \end{pmatrix} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix} \qquad \frac{T\beta}{m} < 2$$

Symplectic methods

If $\det K(y) = K_1 K_4 - K_2 K_3 = 1$ then

$$\begin{pmatrix} K_1^{2k-2} & K_2^{2k-1} \\ K_3^{2k-1} & K_4^{2k} \end{pmatrix}$$
$$= \begin{pmatrix} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{pmatrix} \begin{pmatrix} K_1^{2(k-1)-2} & K_2^{2(k-1)-1} \\ K_3^{2(k-1)-1} & K_4^{2(k-1)} \end{pmatrix}$$

If the solution exists, it is unique and trivial to obtain.

Symplectic methods

If $\det K(y) = K_1 K_4 - K_2 K_3 = 1$ then

$$\begin{pmatrix} K_1^{2k-2} & K_2^{2k-1} \\ K_3^{2k-1} & K_4^{2k} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{pmatrix} \begin{pmatrix} K_1^{2(k-1)-2} & K_2^{2(k-1)-1} \\ K_3^{2(k-1)-1} & K_4^{2(k-1)} \end{pmatrix}$$

If the solution exists, it is unique and trivial to obtain.
In addition

$$\begin{pmatrix} K_1 & K_2 \\ K_3 & K_4 \end{pmatrix} = Q^{-1} \begin{pmatrix} \cos(\phi(y)) & \sin(\phi(y)) \\ -\sin(\phi(y)) & \cos(\phi(y)) \end{pmatrix} Q$$

with $\phi(y) = \arccos(\frac{1}{2}(K_1 + K_4))$

Symplectic methods

$$K(y)^n \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} = O(n\phi(y)) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} + E(y) \begin{pmatrix} \sin(n\phi(y))q_0 \\ \sin(n\phi(y))p_0 \end{pmatrix}$$

with

$$E(y) = \begin{pmatrix} \epsilon(y) & \gamma(y) - 1 \\ -\dfrac{1+\epsilon(y)^2}{\gamma(y)} + 1 & -\epsilon(y) \end{pmatrix}$$

and

$$\epsilon(y) = \frac{K_1(y) - K_4(y)}{2\sin(\phi(y))}, \qquad \gamma(y) = \frac{K_2(y)}{\sin(\phi(y))}.$$

Symplectic methods

$$\|u(n\tau) - u_n\| \leq (n\mu(\theta) + \nu(\theta)) \|u_0\|$$

where

$$\mu(\theta) = \sup_{0 \leq y \leq \theta} |\phi(y) - y|, \qquad \nu(\theta) = \sup_{0 \leq y \leq \theta} \|E(y)\|.$$

Symplectic methods

$$\|u(n\tau) - u_n\| \le (n\mu(\theta) + \nu(\theta)) \|u_0\|$$

where

$$\mu(\theta) = \sup_{0 \le y \le \theta} |\phi(y) - y|, \qquad \nu(\theta) = \sup_{0 \le y \le \theta} \|E(y)\|.$$

m	θ'	$\sum_j(\lvert a_j\rvert + \lvert b_j\rvert)$	$\mu(\theta)$	$\nu(\theta)$
10	1	4.02	0.00093	0.037
20	1	3.05	0.00061	0.025
30	1	3.19	0.000084	0.037
30	1.4	3.09	0.000051	0.013
30	1	3.04	$2.9 \cdot 10^{-13}$	$2.3 \cdot 10^{-9}$
30	0.75	3.44	$1.2 \cdot 10^{-17}$	$5.9 \cdot 10^{-14}$
30	0.5	3.84	$7.9 \cdot 10^{-24}$	$6.6 \cdot 10^{-18}$
40	1	3.21	$1.1 \cdot 10^{-15}$	$1.0 \cdot 10^{-12}$

- S. Blanes, F. Casas and A. Murua, On the linear stabylity of splitting methods, Found. Comp. Math., 8 (2008), pp. 357-393.
- S. Blanes, F. Casas, and A. Murua, Error analysis of splitting methods for the time dependent Schrodinger equation, SIAM J. Sci. Comput. 33 (2011), pp. 1525-1548
- S. Blanes, F. Casas, and A. Murua. Work in progress

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Schrödinger Equation with Poschl-Teller Potential

The one-dimensional problem

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)$$

with

$$V(x) = -\frac{\alpha^2}{2\mu}\frac{\lambda(\lambda-1)}{\cosh^2(\alpha x)}$$

$\mu = 1745, \quad \alpha = 2, \quad \lambda = 24.5,$
initial conditions

$$\psi(x,0) = \rho \mathrm{e}^{-9^2 x^2}$$

$$t \in [0, T], \quad x \in [-5, 5], \quad \Delta x = 10/N$$

$$E_{min} = V_{min}(x), \quad E_{max} = \frac{1}{2m}\left(\frac{\pi}{\Delta x}\right)^2 + V_{max}(x)$$

$$\beta = \frac{E_{max} - E_{min}}{2}$$

N	64	128	256	512	1024
β	0.387	0.561	1.25	4.03	15.1

T	15π	3π
tol	10^{-8}	10^{-12}

$$t \in [0, T], \quad x \in [-5, 5], \quad \Delta x = 10/N$$

$$E_{min} = V_{min}(x), \quad E_{max} = \frac{1}{2m}\left(\frac{\pi}{\Delta x}\right)^2 + V_{max}(x)$$

$$\beta = \frac{E_{max} - E_{min}}{2}$$

N	64	128	256	512	1024
β	0.387	0.561	1.25	4.03	15.1

T	15π	3π
tol	10^{-8}	10^{-12}

	Taylor	Chebyshev	Symplectic
$T\,\beta = 26.3$ $tol = 10^{-8}$	**118** $1.5 \cdot 10^{-15}$	**50** $1.6 \cdot 10^{-11}$	**30** $1.3 \cdot 10^{-10}$
$T\,\beta = 37.9$ $tol = 10^{-12}$	**208** $1.3 \cdot 10^{-13}$	**73** $2.5 \cdot 10^{-15}$	**40** $4.7 \cdot 10^{-14}$

Conclusions

We have shown how to build a class of methods for the Schrödinger equation following the steps previously mentioned:

1. We have define mathematically the physical problem
2. We have reviewed the The State of the Art on methods to solve the problem
3. We have used our knowledge on the physical problem, scientific computation, abstract and applied algebra, functional analysis, optimization, etc. to improve the existing methods

Future Work

1. To develop a fast and automatic algorithm which finds the optimal coefficients for each particular problem
2. To develop new methods when additional information on the problem is known: e.g. If $\|H^k u_0\| \ll \|H\|^k \cdot \|u_0\|$.
3. To extend the methods to problems with similar structure: Maxwell Equations or some linear Hyperbolic PDEs

Thank You

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Numerical Solution of Differential and Differential-Algebraic Equations
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Halle (Saale), Germany