Splitting Methods for Oscillatory non-autonomous linear systems

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Effective Computational Methods for Highly Oscillatory Solutions

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Joint work with Fernando Casas and Ander Murua

Introduction

Problem: To numerically solve the linear time dependent system

$$x' = M(t)y, \qquad y' = -N(t)x$$

with $x(t_0) = x_0 \in \mathbb{R}^{d_1},\ y(t_0) = y_0 \in \mathbb{R}^{d_2} \quad d_1, d_2 \gg 1$

They can appear after discretisation of linear PDEs (or their linear part): linear and non-linear Schrödinger equation, Maxwell equations, etc.

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Constraints for our problems: to build numerical methods which only involve matrix-vector products, i.e. $M(t_i)y, \quad N(t_i)x$

or $\bar{M}_i y, \quad \bar{N}_i x$

with $$\bar{M}_i = \sum_{j=1}^{k} \rho_{ij} M(t_j), \qquad \bar{N}_i = \sum_{j=1}^{k} \sigma_{ij} N(t_j)$$

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For the autonomous case, if we denote $z=(x,y)^T$

$$z' = \big(A+B\big)z \quad \text{where} \quad A = \begin{pmatrix} 0 & M \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ -N & 0 \end{pmatrix}$$

The formal solution is well known for this problem

$$z(t) = e^{t(A+B)}z(0)$$

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Notice that

$$e^{tA} = \begin{pmatrix} I & tM \\ 0 & I \end{pmatrix}, \; e^{tB} = \begin{pmatrix} I & 0 \\ -tN & I \end{pmatrix}$$

and $[\mathbf{A},[\mathbf{A},[\mathbf{A},\mathbf{B}]]] = [\mathbf{B},[\mathbf{B},[\mathbf{B},\mathbf{A}]]] = 0$

We can use this information to build splitting methods

$$M(h) \equiv \prod_{i=1}^{m} e^{ha_i A} \, e^{hb_i B}$$

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The simplest solution is to convert the system into autonomous

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We consider the **Magnus series expansion** to obtain the formal solution up to a given order in the time step

Then, we approximate this formal solution using the techniques developed for splitting methods

The Schrödinger Equation

Consider the linear time dependent SE

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

The solution of the discretised equation is given by

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

where $\mathbf{c} = (c_1,\ldots, c_N)^T \in \mathbb{C}^N$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{R}^{N\times N}$ Hermitian matrix.
Fourier methods are frequently used

$$(\mathbf{V}\mathbf{c})_i = V(x_i)c_i \qquad N \text{ products}$$

$$\mathbf{T}\mathbf{c} = \mathcal{F}^{-1}\mathbf{D}_T\,\mathcal{F}\mathbf{c} \qquad \mathcal{O}(N\log N) \text{ operations}$$

$\mathcal{F}$ is the fast Fourier transform (FFT)

The Schrödinger Equation

Some Methods which mainly require products $\mathbf{Hc}$: Chebishev, iterative Lanczos, second order differencing scheme, unitary split operator, **symplectic split operators**

The problem to solve is

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

If we consider $\mathbf{c} = \mathbf{q} + i\mathbf{p}$ then $i\frac{d}{dt}(\mathbf{q} + i\mathbf{p}) = \mathbf{H}(\mathbf{q} + i\mathbf{p})$

Equivalent to the classical Hamiltonian system: $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q}$

$$\frac{d}{dt}\left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\} = \left(\begin{array}{cc} 0 & \mathbf{H} \\ -\mathbf{H} & 0 \end{array} \right) \left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\}$$

and symplectic integrators can be used

The Schrödinger Equation

Let us denote $\mathbf{z} = (\mathbf{q}, \mathbf{p})^T$ then

$$\mathbf{z}' = (\mathbf{A} + \mathbf{B})\mathbf{z}, \quad \mathbf{A} = \begin{pmatrix} 0 & \mathbf{H} \\ 0 & 0 \end{pmatrix}, \; \mathbf{B} = \begin{pmatrix} 0 & 0 \\ -\mathbf{H} & 0 \end{pmatrix}$$

with formal solution

$$\mathbf{O}(t) = e^{t(\mathbf{A}+\mathbf{B})} = \begin{pmatrix} \cos(t\mathbf{H}) & \sin(t\mathbf{H}) \\ -\sin(t\mathbf{H}) & \cos(t\mathbf{H}) \end{pmatrix}$$

It is an orthogonal and symplectic operator.

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Since $$e^{\mathbf{A}} = \begin{pmatrix} \mathbf{I} & \mathbf{H} \\ 0 & \mathbf{I} \end{pmatrix}, \; e^{\mathbf{B}} = \begin{pmatrix} \mathbf{I} & 0 \\ -\mathbf{H} & \mathbf{I} \end{pmatrix}$$

we can use splitting methods to numerically approximate $\mathbf{O}(t)$, i.e.
Störmer/Strang//Verlet/leap-frog

$$\mathbf{z}_i = e^{\tau \mathbf{A}/2} \, e^{\tau \mathbf{B}} \, e^{\tau \mathbf{A}/2} \mathbf{z}_{i-1} \quad \Rightarrow \quad \left\{ \begin{array}{rcl} \bar{\mathbf{q}} & = & \mathbf{q}_{i-1} + \tau \mathbf{H} \mathbf{p}_i/2 \\ \mathbf{p}_i & = & \mathbf{p}_{i-1} - \tau \mathbf{H} \bar{\mathbf{q}} \\ \mathbf{q}_i & = & \bar{\mathbf{q}} + \tau \mathbf{H} \mathbf{p}_i/2 \end{array} \right.$$

Remember that $$\boxed{[\mathbf{A}, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]] = [\mathbf{B}, [\mathbf{B}, [\mathbf{B}, \mathbf{A}]]] = 0}$$

The Schrödinger Equation

We denote the second order method by

$$\mathrm{U}_2(\tau) \equiv e^{\tau \mathrm{A}/2}\, e^{\tau \mathrm{B}}\, e^{\tau \mathrm{A}/2}$$

with associated algorithm

$$\begin{cases} \bar{\mathbf{q}} &= \mathbf{q}_{i-1} + \tau \mathbf{H} \mathbf{p}_i/2 \\ \mathbf{p}_i &= \mathbf{p}_{i-1} - \tau \mathbf{H} \bar{\mathbf{q}} \\ \mathbf{q}_i &= \bar{\mathbf{q}} + \tau \mathbf{H} \mathbf{p}_i/2 \end{cases}$$

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$$\begin{aligned} \mathbf{H}\mathbf{c} &= (\mathbf{T} + \mathbf{V})\,\mathbf{c} \\ &= \left(\mathcal{F}^{-1} \mathbf{D}_T\, \mathcal{F} + \mathbf{V}\right) \mathbf{c} \end{aligned}$$

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algorithm

```
% Starting
do  l = 1, M
    q = q + τH · p/2
    p = p − τH · q
    q = q + τH · p/2
enddo

sub(Hy)
    do  j = 0, N − 1
        v_j = V(x_j)/2
        t_j = D_Tj
    enddo
    y2 = v · y
    call FFT(c)
    y1 = t · c
    call invFFT(y1)
    c = y1 + y2
enddo
```

Higher Orders

The well known fourth-order composition scheme

$$\mathbf{U}_4(h) = \mathbf{U}_2(\alpha_1 h)\mathbf{U}_2(\alpha_0 h)\mathbf{U}_2(\alpha_1 h)$$

with

$$\alpha_1 = \frac{1}{2 - 2^{1/3}}, \quad \alpha_0 = 1 - 2\alpha_1$$

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Or in general

$$\mathrm{U}_{2n+2}(h) = \mathrm{U}_{2n}^p(\alpha_1 h)\mathrm{U}_{2n}(\alpha_0 h)\mathrm{U}_{2n}^p(\alpha_1 h)$$

with

$$\alpha_1 = \frac{1}{2p - (2p)^{1/(2n+1)}}, \quad \alpha_0 = 1 - 2\alpha_1$$

-Creutz-Gocksh(89)
-Suzuki(90)
-Yoshida(90)

Splitting Methods

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$$\begin{aligned} \mathbf{U}_n(h) &= e^{hb_k \mathbf{B}}\, e^{ha_k \mathbf{A}} \;\cdots\; e^{hb_1 \mathbf{B}}\, e^{ha_1 \mathbf{A}} \\ &= \Phi_1^*(d_k h)\Phi_1(c_k h) \;\cdots\; \Phi_1^*(d_1 h)\Phi_1(c_1 h) \end{aligned}$$

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$$\mathrm{U}_n(h) = e^{hb_k \mathbf{H}_0}\, e^{\epsilon h a_k \mathbf{H}_1} \ \ldots\ e^{hb_1 \mathbf{H}_0}\, e^{\epsilon h a_1 \mathbf{H}_1}$$

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$$\mathrm{U}_n = \mathrm{U}_P \mathrm{U}_K \mathrm{U}_P^{-1} \quad \Longrightarrow \quad \mathrm{U}_n^p = \mathrm{U}_P \mathrm{U}_K^p \mathrm{U}_P^{-1}$$

Numerical Example

Schrödinger equation with a Morse potential

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

with

$$V(x) = D(1 - e^{-\alpha x})^2$$

$$\mu = 1745,\ D = 0.2251,\ \alpha = 1.1741$$

Initial conditions

$$\psi(x,t) = \rho \exp\left(- \beta(x - x_m)^2\right)$$

$$\beta = \sqrt{D\mu\alpha^2/2},\ \bar{x} = -0.1 \quad (\rho \text{ norm. const.})$$

$$t \in [0, 500\,T] \quad \text{with} \quad T = 2\pi/\left(\alpha\sqrt{2D/\mu}\right)$$

$$x \in [-0.8, 4.32], \text{ split into } N = 64 \text{ parts}$$

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Perturbation of the Morse potential with a laser field

$$V_I(x,t) = A\cos(\omega t)x$$

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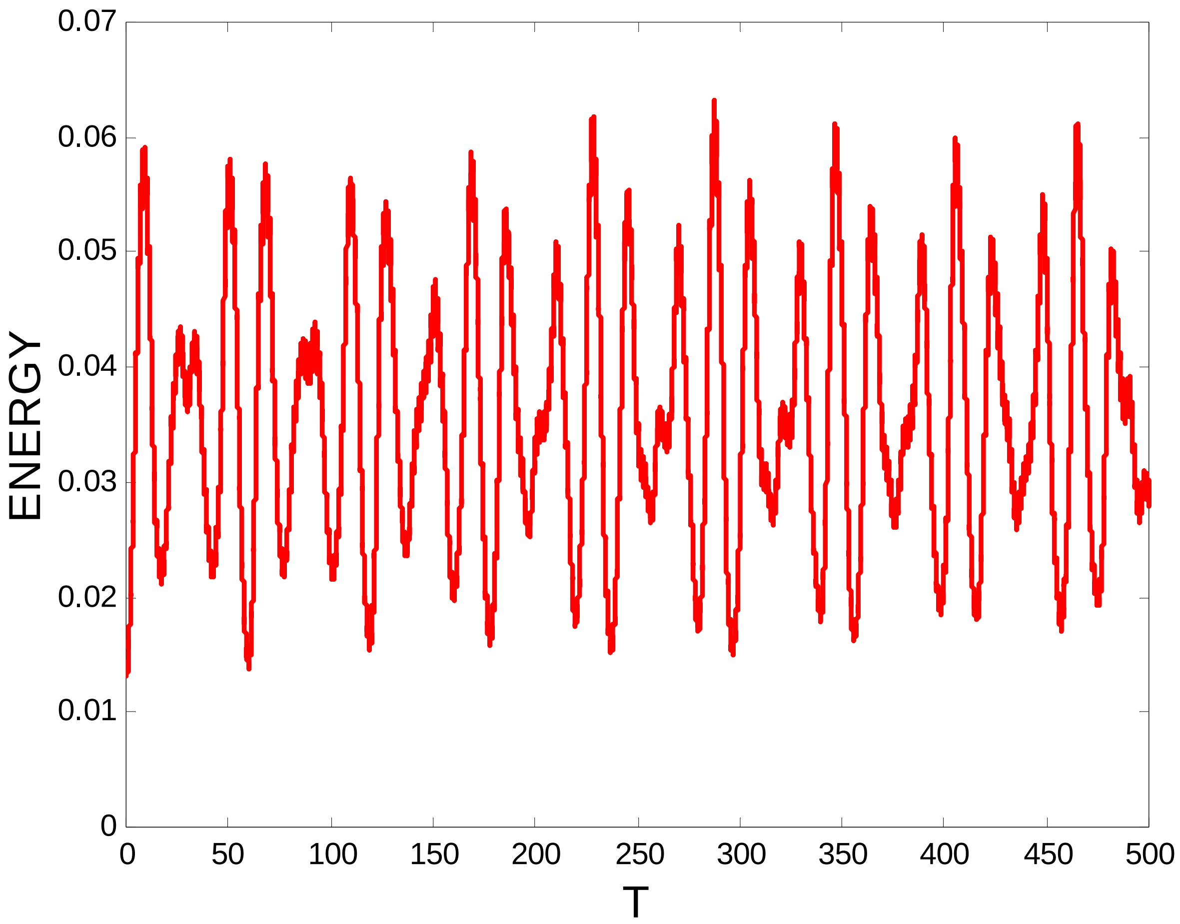

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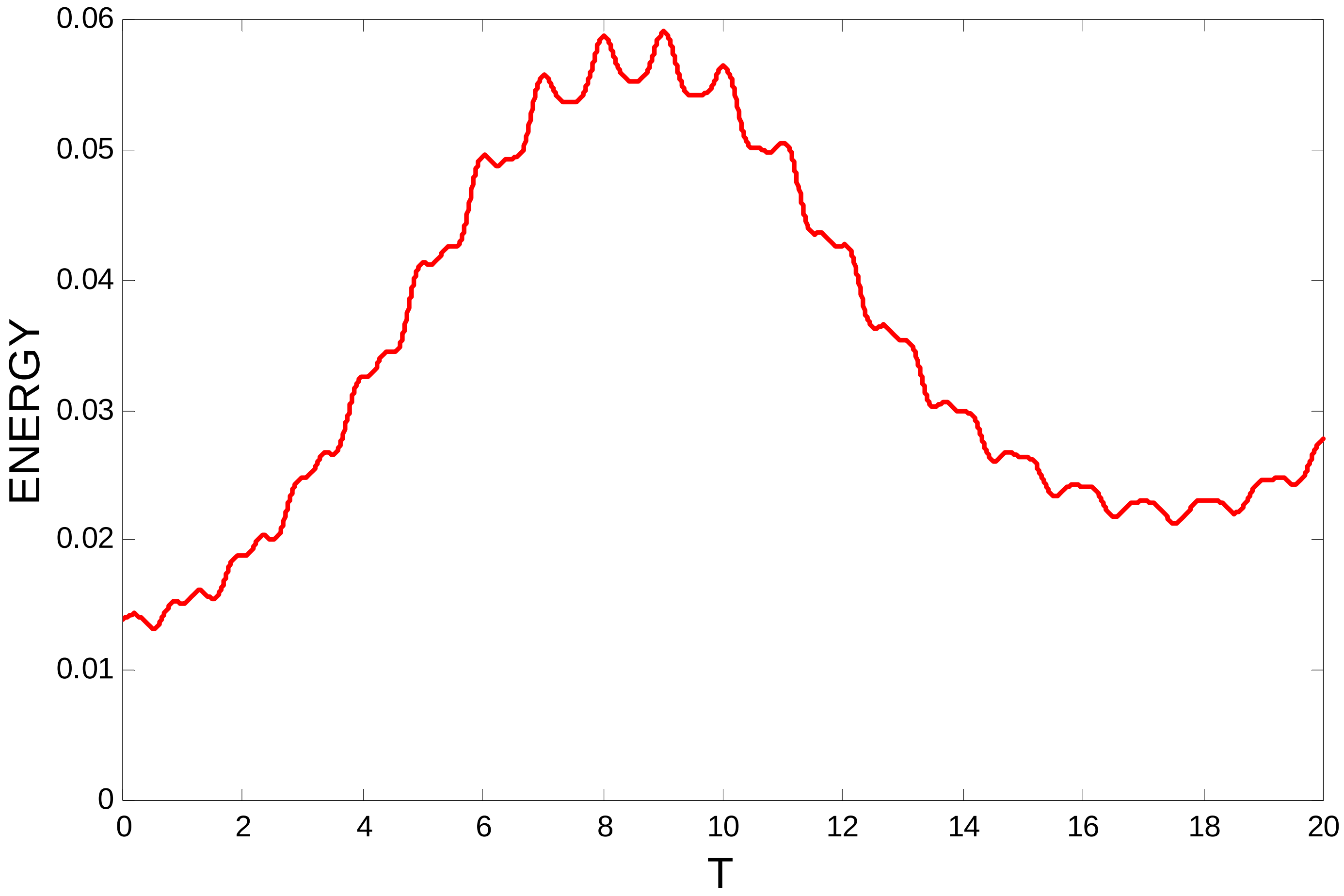
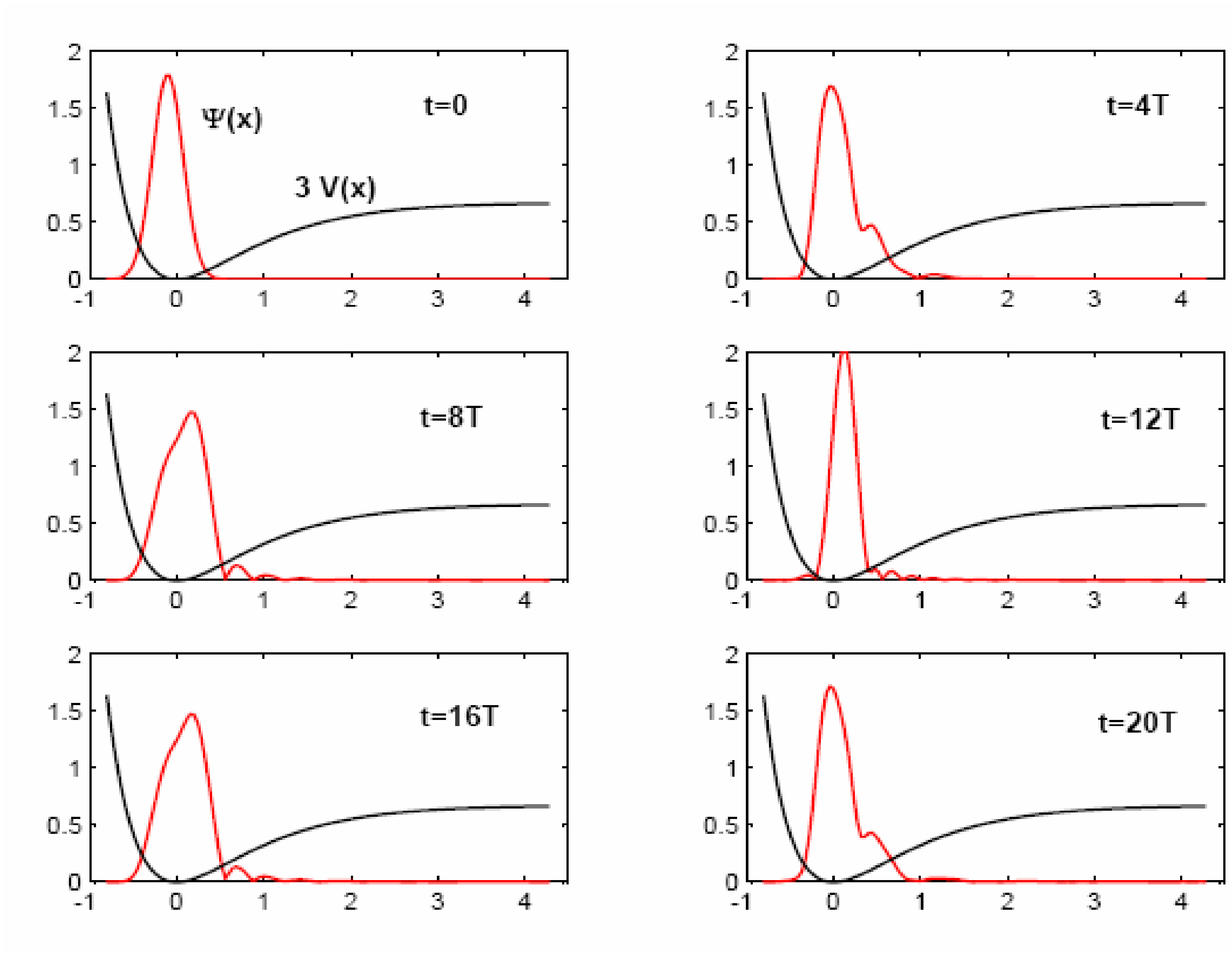


Numerical Example

Gaussian wave fuction in a Morse potential



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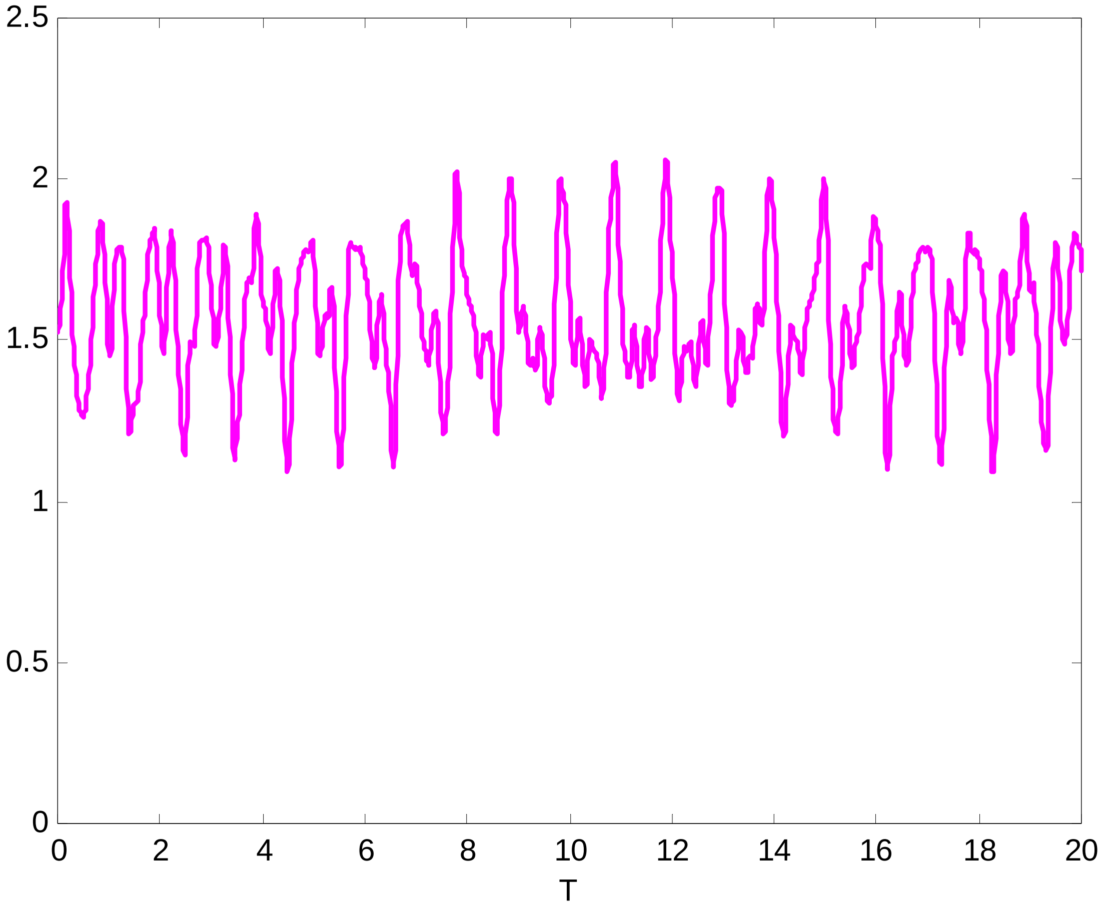

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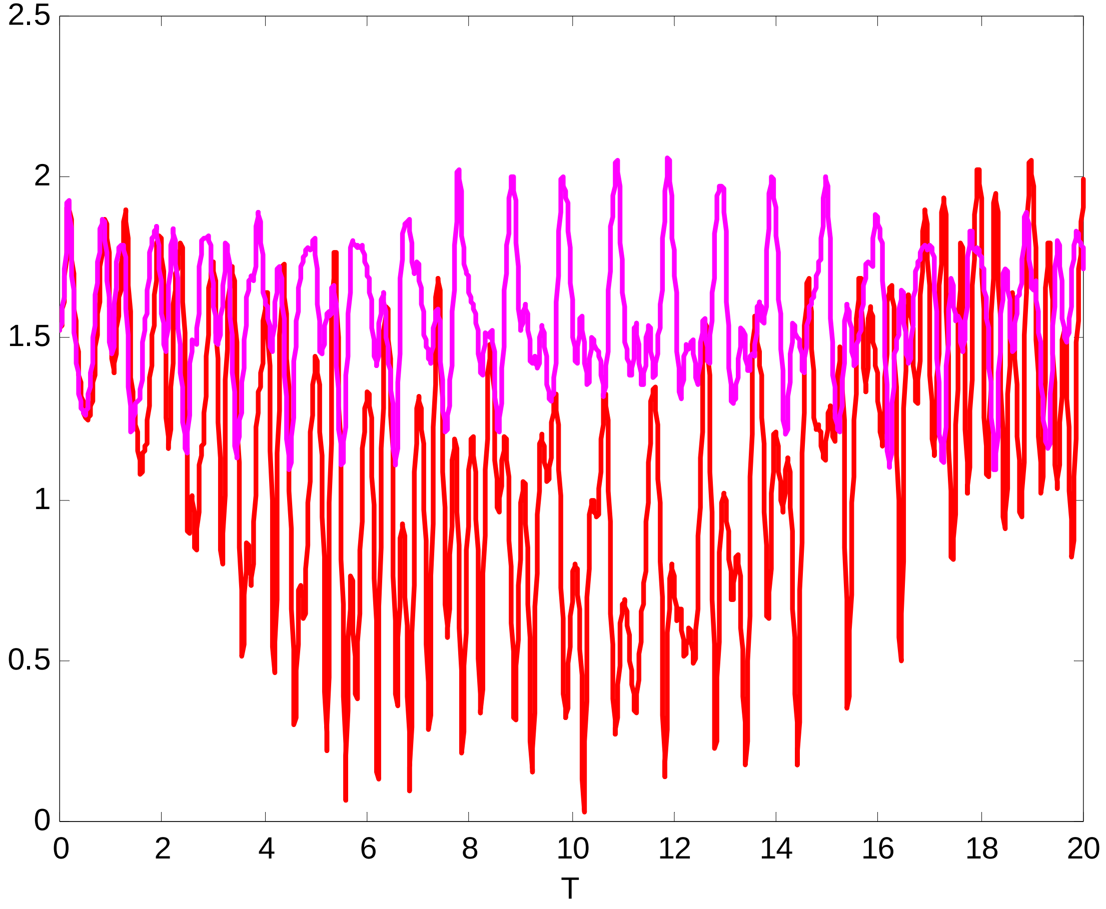

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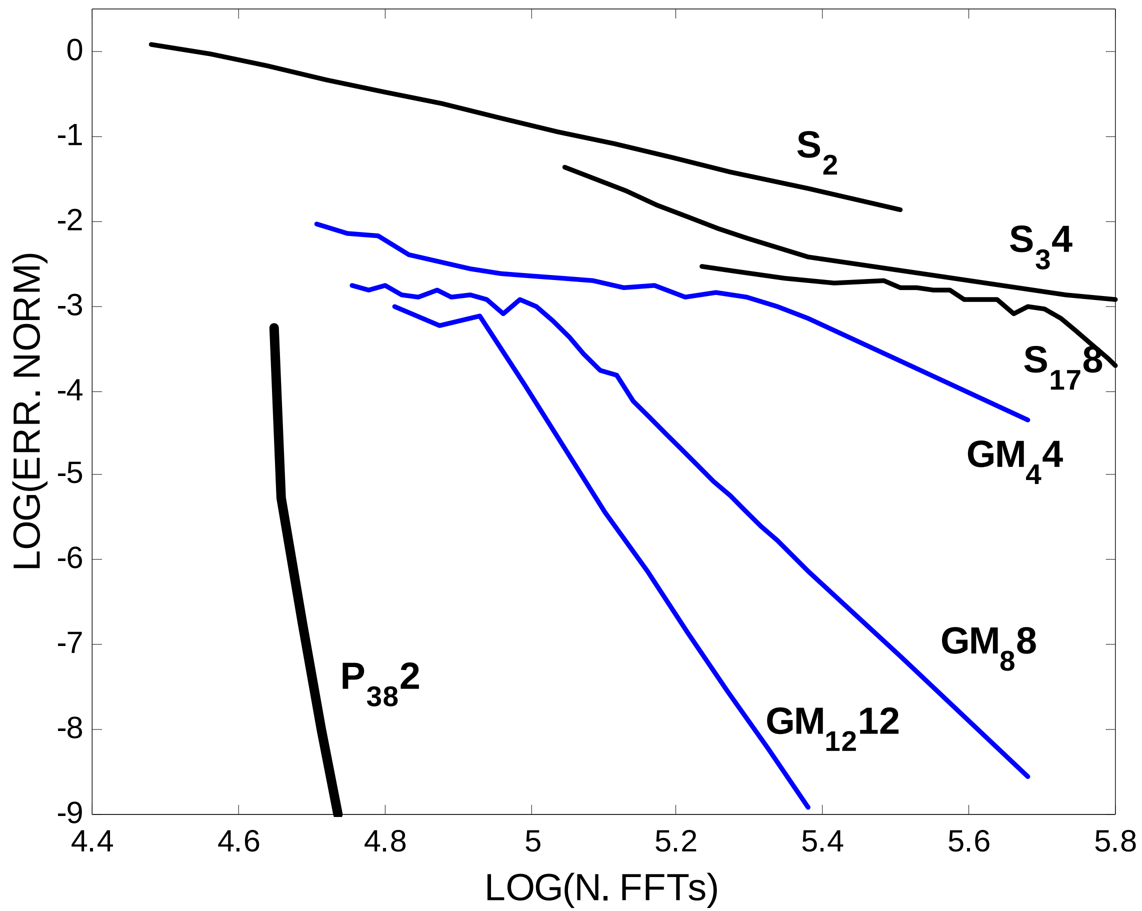

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with $$\bar{M}_i = \sum_{j=1}^{k} \rho_{ij} M(t_j), \qquad \bar{N}_i = \sum_{j=1}^{k} \sigma_{ij} N(t_j)$$

Let us consider $z = (x, y)^T$ then

$$z' = \big(A(t) + B(t)\big)z$$

with

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Since $e^{A_i(t,h)} = \begin{pmatrix} I & M_i(t,h) \\ 0 & I \end{pmatrix}, \quad e^{B_i(t,h)} = \begin{pmatrix} I & 0 \\ -N_i(t,h) & I \end{pmatrix}$

with $M_i = h \sum_{j=1}^{k} \rho_{ij} M(t + c_j h), \quad N_i = h \sum_{j=1}^{k} \sigma_{ij} N(t + c_j h)$

can be computed efficiently, we analyse the following compositions

$$K(t,h) = e^{A_m(t,h)} e^{B_m(t,h)} \cdots e^{A_1(t,h)} e^{B_1(t,h)}$$

$$= \begin{pmatrix} I & M_m \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_m & I \end{pmatrix} \cdots \begin{pmatrix} I & M_1 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_1 & I \end{pmatrix}$$

How to choose the parameters $c_i, \rho_{ij}, \sigma_{ij}$?

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$$= \begin{pmatrix} I & a_m hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_m hN & I \end{pmatrix} \cdots \begin{pmatrix} I & a_1 hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_1 hN & I \end{pmatrix}$$

and then

$$a_i = \sum_{j=1}^{k} \rho_{ij}, \qquad b_i = \sum_{j=1}^{k} \sigma_{ij}, \qquad i = 1, \ldots, m$$

Then, it is important to start with the coefficients a_i , b_i from an efficient splitting method for the autonomous case.

How to choose the parameters $c_i, \rho_{ij}, \sigma_{ij}$?

In the autonomous case we have

$$K(h) = e^{ha_m A} e^{hb_m B} \cdots e^{ha_1 A} e^{hb_1 B}$$

$$= \begin{pmatrix} I & a_m hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_m hN & I \end{pmatrix} \cdots \begin{pmatrix} I & a_1 hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_1 hN & I \end{pmatrix}$$

and then

$$a_i = \sum_{j=1}^{k} \rho_{ij}, \qquad b_i = \sum_{j=1}^{k} \sigma_{ij}, \qquad i = 1, \ldots, m$$

Then, it is important to start with the coefficients a_i , b_i from an efficient splitting method for the autonomous case.

At this point, to proceed further, we need to know the formal solution. Then we consider the **Magnus series expansion**

Magnus series expansion

$$z(t+h) = e^{\Omega(t,h)} z(t) \quad \text{where} \quad \Omega(t,h) = \sum_{k=1}^{\infty} \Omega_k(t,h)$$

and

$$\begin{aligned}
\Omega_1 &= \int_t^{t+h} (A(t) + B(t))dt \\
\Omega_2 &= \frac{1}{2}\int_t^{t+h} dt_1 \int_t^{t_1} dt_2 [A(t_1) + B(t_1), A(t_2) + B(t_2)] \\
&\vdots
\end{aligned}$$

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We work in the bi-gradded Lie algebra generated by

$$\alpha_i = \frac{1}{(i-1)!} \frac{d^{i-1} A(s)}{ds^{i-1}}\Big|_{s=t+\frac{h}{2}} \qquad \beta_i = \frac{1}{(i-1)!} \frac{d^{i-1} B(s)}{ds^{i-1}}\Big|_{s=t+\frac{h}{2}}$$

$$\begin{aligned}
A(t + \tfrac{h}{2} + \tau) &= \alpha_1 + \alpha_2 \tau + \alpha_3 \tau^2 + \cdots \\
B(t + \tfrac{h}{2} + \tau) &= \beta_1 + \beta_2 \tau + \beta_3 \tau^2 + \cdots
\end{aligned}$$

Magnus series expansion

We rewrite the series

$$\Omega = \sum_{k=1}^{\infty} \Omega_k = \sum_{n\geq 1} h^n \sum_{k=1}^{n} \Omega_{k,n}$$

i.e.

$$\begin{aligned}\Omega \;=\; & h\Omega_{1,1} + h^3(\Omega_{1,3} + \Omega_{2,3}) \\ & + h^5(\Omega_{1,5} + \Omega_{2,5} + \Omega_{3,5} + \Omega_{4,5}) + \mathcal{O}(h^7)\end{aligned}$$

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where
$$\begin{aligned}\Omega_{1,1} &= \alpha_1 + \beta_1, \qquad \Omega_{1,3} = \frac{1}{12}(\alpha_3 + \beta_3) \\ \Omega_{1,5} &= \frac{1}{80}(\alpha_5 + \beta_5), \qquad \Omega_{2,3} = \frac{1}{12}([\alpha_2, \beta_1] + [\beta_2, \alpha_1]) \\ \Omega_{2,5} &= \frac{1}{240}([\alpha_2, \beta_3] + [\beta_2, \alpha_3]) + \frac{1}{80}([\alpha_4, \beta_1] + [\beta_4, \alpha_1]) \\ \Omega_{3,5} &= \frac{1}{360}\big(- [\alpha_1, \beta_3, \alpha_1] + \cdots \big) + \cdots \\ & \vdots\end{aligned}$$

Remember we were looking for a composition like

$$K(t,h) = e^{A_m(t,h)} e^{B_m(t,h)} \dots e^{A_1(t,h)} e^{B_1(t,h)}$$

where

$$A_i(t,h) = h \sum_{j=1}^{k} \rho_{ij} A(t + c_j h), \qquad B_i(t,h) = h \sum_{j=1}^{k} \sigma_{ij} B(t + c_j h)$$

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and we look for the coefficients $a_i^{(n)}, b_i^{(n)}$ but starting from an efficient splitting method. Finally, it is easy to show that

$$\rho_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} a_i^{(n)} r_{nl} d_j (c_j - \frac{1}{2})^{l-1}, \qquad \sigma_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} b_i^{(n)} r_{nl} d_j (c_j - \frac{1}{2})^{l-1}$$

where the coefs. d_j, c_j are the weights and nodes of any sixth order quadrature and

$$(r_{n,l}) = \begin{pmatrix} \frac{9}{4} & 0 & -15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix}$$

Numerical Example

Gaussian wave fuction in a Morse potential

with laser field $V_I(x,t) = A\cos(\omega t)x$

$A = 0{,}011025$

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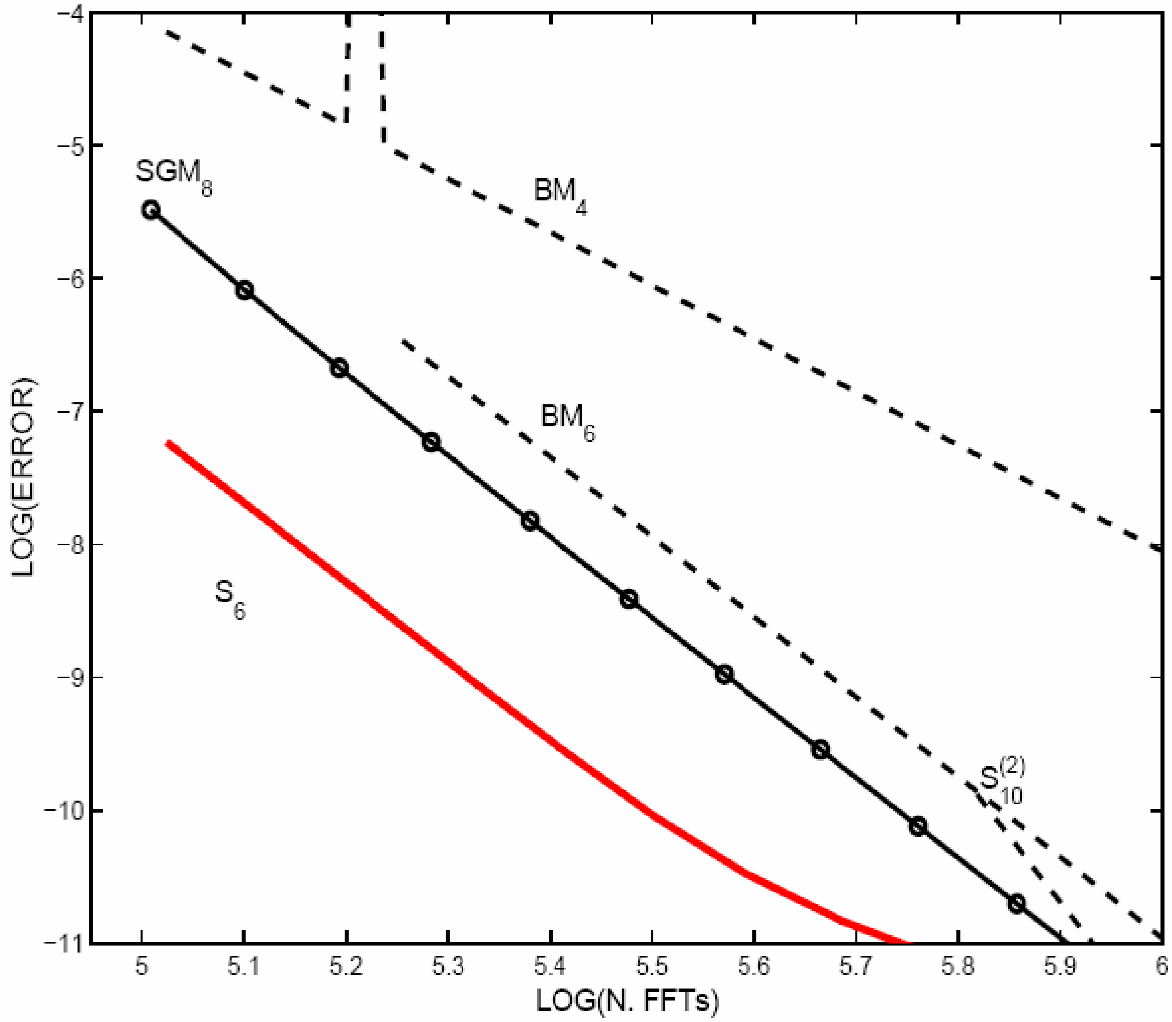

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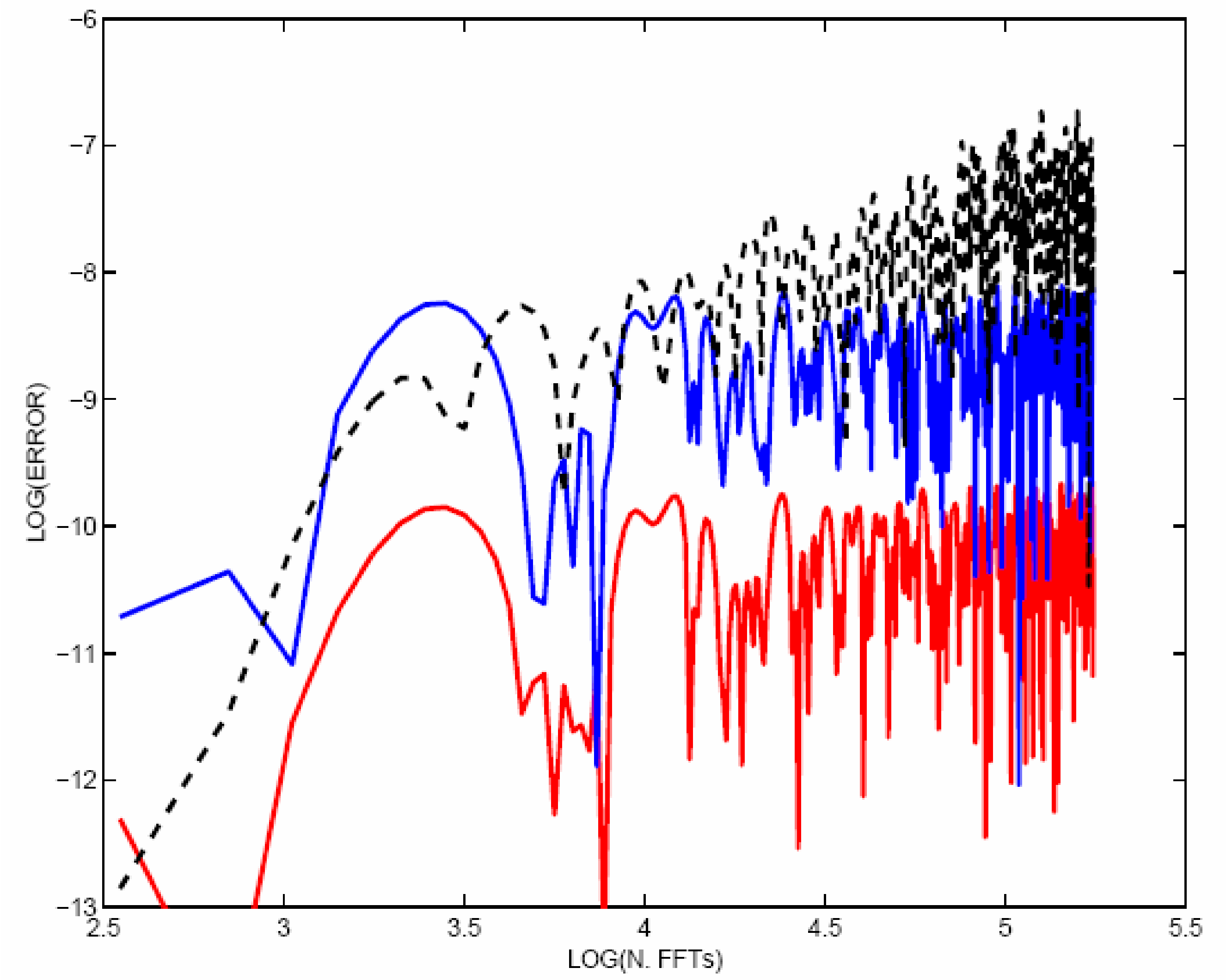

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Splitting Methods for Oscillatory non-autonomous linear systems

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Effective Computational Methods for Highly Oscillatory Solutions

Cambridge, 2-6 July 2007

Joint work with Fernando Casas and Ander Murua

Problem to Solve: To build splitting methods for the harmonic oscillator!!!

$$\frac{d}{dt}\left\{\begin{array}{c} q \\ p \end{array}\right\} = \Bigg[\underbrace{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}}_{B}\Bigg]\left\{\begin{array}{c} q \\ p \end{array}\right\}$$

Exact solution

$$O(t) = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix}$$

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Notice that

$$e^{hA}\, e^{hB} = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix} = \begin{pmatrix} 1-h^2 & h \\ -h & 1 \end{pmatrix}$$

Let us consider the composition

$$M(h) \equiv \prod_{i=1}^{m} e^{h a_i A}\, e^{h b_i B}$$

$$\equiv \prod_{i=1}^{m} \begin{pmatrix} 1 - a_i b_i h^2 & a_i h \\ -b_i h & 1 \end{pmatrix} = \begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix}$$