The Magnus expansion and its physical applications

Fernando Casas
Fernando.Casas@mat.uji.es
www.gicas.uji.es

Departament de Matemàtiques
Universitat Jaume I
Castellón, Spain

Barcelona, 24 March 2009

Based on the review paper

The Magnus expansion and some of its applications, Physics Reports **470** (2009), 151-238

by

S. Blanes
Universidad Politécnica de Valencia
Valencia, Spain

J.A. Oteo, J. Ros
Universitat de València
Valencia, Spain

and F. C.

Supported by MEC (Spain), project MTM2007-61572

Time-dependent Schrödinger equation

... with a time-dependent potential

$$i\frac{\partial}{\partial t}\psi(t,x) = \hat{H}(t)\psi(t,x) \equiv \left(\hat{T} + \hat{V}(t)\right)\psi(t,x), \qquad (1)$$

where

$$\hat{T}\psi \equiv -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}, \qquad \hat{V}(t)\psi \equiv \left(V(x) + \tilde{V}(t,x)\right)\psi.$$

Problem: Solve the equation!

Approach 1. Suppose $\{E_n, \varphi_n\}_{n=0}^{\infty}$ is a complete set of eigenvalues and eigenvectors for $\hat{H}$ when $\tilde{V}(t,x) \equiv 0$. Then an approximate solution can be obtained as

$$\psi(t,x) \simeq \sum_{n=0}^{d-1} c_n(t)\,\mathrm{e}^{-itE_n}\,\varphi_n(x). \qquad (2)$$

Time-dependent Schrödinger equation

... with a time-dependent potential

$$i\frac{\partial}{\partial t}\psi(t,x) = \hat{H}(t)\psi(t,x) \equiv \left(\hat{T} + \hat{V}(t)\right)\psi(t,x), \qquad (1)$$

where

$$\hat{T}\psi \equiv -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}, \qquad \hat{V}(t)\psi \equiv \left(V(x) + \tilde{V}(t,x)\right)\psi.$$

Problem: Solve the equation!

Approach 1. Suppose $\{E_n, \varphi_n\}_{n=0}^{\infty}$ is a complete set of eigenvalues and eigenvectors for $\hat{H}$ when $\tilde{V}(t,x) \equiv 0$. Then an approximate solution can be obtained as

$$\psi(t,x) \simeq \sum_{n=0}^{d-1} c_n(t)\,\mathrm{e}^{-itE_n}\,\varphi_n(x). \qquad (2)$$

Time-dependent Schrödinger equation

Substituting (2) into (1) we obtain the matrix equation

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}(t)\,\mathbf{c}(t), \qquad \mathbf{c}(0) = \mathbf{c}_0, \tag{3}$$

where $\mathbf{c} = (c_0, \ldots, c_{d-1})^T \in \mathbb{C}^d$, $\mathbf{H} \in \mathbb{C}^{d\times d}$ is an Hermitian matrix such that

$$(\mathbf{H}(t))_{ij} = \langle\varphi_i|\hat{H}(t) - \hat{H}_0|\varphi_j\rangle\, \mathrm{e}^{i(E_i-E_j)t}, \qquad i,j = 1,\ldots,d$$

and $\hat{H}_0 = \hat{H}(t=0)$.
d depends on the problem, the accuracy required, etc.
Galerkin-like procedure

Time-dependent Schrödinger equation

Substituting (2) into (1) we obtain the matrix equation

$$i\,\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}(t)\,\mathbf{c}(t), \qquad \mathbf{c}(0) = \mathbf{c}_0, \tag{3}$$

where $\mathbf{c} = (c_0, \ldots, c_{d-1})^T \in \mathbb{C}^d$, $\mathbf{H} \in \mathbb{C}^{d\times d}$ is an Hermitian matrix such that

$$(\mathbf{H}(t))_{ij} = \langle \varphi_i | \hat{H}(t) - \hat{H}_0 | \varphi_j \rangle \, \mathrm{e}^{i(E_i - E_j)t}, \qquad i,j = 1, \ldots, d$$

and $\hat{H}_0 = \hat{H}(t=0)$.
d depends on the problem, the accuracy required, etc.
Galerkin-like procedure

Time-dependent Schrödinger equation

Approach 2. Space discretization (by collocation methods)

- System defined in the interval $x \in [x_0, x_f]$ with periodic boundary conditions
- Split the interval in d parts of length $\Delta x = (x_f - x_0)/d$ and consider $u_n = \psi(t, x_n)$ where $x_n = x_0 + n\Delta x$, $n = 0, 1, \ldots, d-1$.
- We get a system of differential equations for the grid values u_j of the vector $\mathbf{u} = (u_j)$:

$$i \frac{d}{dt}\mathbf{u}(t) = \mathcal{F}^{-1} D_T \mathcal{F}\mathbf{u} + \hat{V}\mathbf{u} \tag{4}$$

where D_T, $\hat{V}$ are diagonal matrices, $\mathcal{F}$ is the discrete Fourier transform (FFT algorithm)

Time-dependent Schrödinger equation

- One ends up with a linear equation of the form

$$i\frac{d\psi}{dt}(t) = H(t)\psi(t), \qquad \psi(0) = \psi_0 \tag{5}$$

  where $\psi(t)$ represents a complex vector with d components which approximates the (continuous) wave function.
- The computational Hamiltonian $H(t)$ appearing in (5) is thus a space discretization (or other finite-dimensional model) of $\hat{H}(t) = \hat{T} + \hat{V}(t)$.
- Numerical difficulties come mainly from the unbounded nature of the Hamiltonian and the highly oscillatory behaviour of the wave function.
- Different computational strategies. More on this in, e.g., J. Geiser and S. Blanes talks.

Time-independent Schrödinger equation

- Goal: compute the discrete eigenvalues defined by the problem

$$-\frac{d^2\varphi}{dx^2} + V(x)\varphi = \lambda\varphi, \qquad x \in (a,b) \tag{6}$$

  with $\varphi(a) = \varphi(b) = 0$
- The problem (6) can be formulated in $\mathrm{SL}(2)$:

$$\frac{d\mathbf{y}}{dx} = \begin{pmatrix} 0 & 1 \\ V(x) - \lambda & 0 \end{pmatrix} \mathbf{y}, \qquad x \in (a,b), \tag{7}$$

  where $\mathbf{y} = (\varphi, d\varphi/dx)^T$.
- Again, the same type of problem

More examples

- Sturm–Liouville problems
- Differential Riccati equation
- Geometric control theory
- Optics (Helmholtz equation)
- ...

General linear equation

Goal

Given the $n \times n$ coefficient matrix $A(t)$, solve the the initial value problem associated with the linear ordinary differential equation

$$Y'(t) = A(t)Y(t), \qquad Y(t_0) = Y_0. \tag{8}$$

- When $n = 1$, the solution reads

$$Y(t) = \exp\left(\int_{t_0}^{t} A(s)ds\right) Y_0. \tag{9}$$

- This is still valid for $n > 1$ if $A(t_1)A(t_2) = A(t_2)A(t_1)$ for any t_1 and t_2. In particular, when A is constant.
- In general, (9) is no longer the solution.

General linear equation

- Usual approach:

$$Y(t) = \mathcal{T}\left(\exp \int_{t_0}^{t} A(s)ds\right)$$

  in terms of the *time-ordering operator* $\mathcal{T}$ introduced by Dyson
- Magnus (1954): construct $Y(t)$ as a *true exponential representation*

The Magnus expansion

- The approach proposed by W. Magnus is to express the solution by means of the exponential of a certain matrix function $\Omega(t, t_0)$,

$$Y(t) = \exp \Omega(t, t_0)\, Y_0 \tag{10}$$

- Ω is subsequently constructed as a series expansion,

$$\Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t). \tag{11}$$

- For simplicity, it is customary to write $\Omega(t) \equiv \Omega(t, t_0)$ and to take $t_0 = 0$.

- First terms:

$$\Omega_1(t) = \int_0^t A(t_1)\,\mathrm{d}t_1,$$
$$\Omega_2(t) = \frac{1}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2\ [A(t_1), A(t_2)] \tag{12}$$
$$\Omega_3(t) = \frac{1}{6}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3\ ([A(t_1), [A(t_2), A(t_3)]] + [A(t_3), [A(t_2), A(t_1)]])$$

  $[A, B] \equiv AB - BA$ is the matrix commutator of A and B.

- $\Omega_1(t)$ coincides exactly with the exponent in the scalar case
- If one insists in having an exponential for $Y(t)$ the exponent has to be corrected.
- The rest of the series (11) provides that correction.

How to obtain it

- Insert $Y(t) = \exp \Omega(t)$ into $Y' = A(t)Y$, $Y(0) = I$
- Differential equation satisfied by Ω:

$$\frac{d\Omega}{dt} = \sum_{n=0}^{\infty} \frac{B_n}{n!} \operatorname{ad}_\Omega^n A, \tag{13}$$

where $\operatorname{ad}_\Omega^0 A = A, \qquad \operatorname{ad}_\Omega^{k+1} A = [\Omega, \operatorname{ad}_\Omega^k A]$,
and B_j are the Bernouilli numbers.

- Apply Picard fixed point iteration:

$$\Omega^{[0]} = O, \qquad \Omega^{[1]} = \int_0^t A(t_1)dt_1,$$

$$\Omega^{[n]} = \int_0^t \left(A(t_1)dt_1 - \frac{1}{2}[\Omega^{[n-1]}, A] + \frac{1}{12}[\Omega^{[n-1]}, [\Omega^{[n-1]}, A]] + \cdots \right)$$

so that $\lim_{n\to\infty} \Omega^{[n]}(t) = \Omega(t)$ near $t = 0$

Magnus expansion generator

- Construct the solution as a series (Magnus series)

$$\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t), \tag{14}$$

- Substitute in (13) and integrate. Then one may build recursively all the terms in (14) through

$$\begin{aligned} S_n^{(j)} &= \sum_{m=1}^{n-j} \left[\Omega_m, S_{n-m}^{(j-1)}\right], \qquad 2 \le j \le n-1 \\ S_n^{(1)} &= \left[\Omega_{n-1}, A\right], \end{aligned}$$

so that

$$\Omega_1 = \int_0^t A(\tau)d\tau, \qquad \Omega_n = \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau)d\tau, \qquad n \ge 2.$$

Magnus expansion generator

- When this recursion is worked out explicitly,

$$\Omega_n(t) = \sum_{j=1}^{n-1} \frac{B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=n-1 \\ k_1\geq 1,\ldots,k_j\geq 1}} \int_0^t \mathrm{ad}_{\Omega_{k_1}(s)} \mathrm{ad}_{\Omega_{k_2}(s)} \cdots \mathrm{ad}_{\Omega_{k_j}(s)} A(s)\, ds$$

- Ω_n is a linear combination of n-fold integrals of $n-1$ nested commutators containing n operators A
- The expression becomes increasingly intricate with n.

Some properties of Magnus expansion

- If $A(t)$ belongs to some Lie algebra $\mathfrak{g}$, then $\Omega(t)$ (and any truncation of the Magnus series) also stays in $\mathfrak{g}$ and therefore $\exp(\Omega) \in \mathcal{G}$, where $\mathcal{G}$ is the Lie group whose corresponding Lie algebra is $\mathfrak{g}$.
  1. Symplectic group in classical mechanics
  2. Unitary group for the Schrödinger equation
- The resulting approximations share important qualitative features with the exact solution (e.g., preservation of the norm, etc.)

Some properties of Magnus expansion

- Time-symmetry: $\Omega(t_f, t_0) = -\Omega(t_0, t_f)$. With the midpoint $t_{1/2} = (t_0 + t_f)/2$ and $t_f = t_0 + h$,

$$\Omega\left(t_{1/2} - \frac{h}{2}, t_{1/2} + \frac{h}{2}\right) = -\Omega\left(t_{1/2} + \frac{h}{2}, t_{1/2} - \frac{h}{2}\right)$$

  and thus Ω does not contain even powers of h. If a Taylor series centered around $t_{1/2}$ is considered for $A(t)$, then $\Omega_{2i+1}\left(t_{1/2} + \frac{h}{2}, t_{1/2} - \frac{h}{2}\right) = \mathcal{O}(h^{2i+3})$.
- Particular case: if $A(t_f - t) = A(t)$, then $\Omega_{2i} \equiv 0$ (problem in quantum computation)

Convergence

- Is this result only formal? What about convergence?
- Specifically, given a certain operator $A(t)$, when $\Omega(t)$ in (10) can be obtained as the sum of the series $\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t)$?
- It turns out that the Magnus series converges for $t \in [0, T)$ such that

$$\int_0^T \|A(s)\| ds < \pi$$

  where $\|\cdot\|$ denotes a matrix norm.
- This result is generic, in the sense that one may consider specific matrices $A(t)$ where the series diverges for any $t > T$.
- ... But it is only a *sufficient* condition: there are matrices $A(t)$ for which the Magnus series converges for $t > T$.

Convergence

Remarks

- Result valid for *complex* matrices $A(t)$
- In fact, if $A(t)$ is any bounded operator on a Hilbert space $\mathcal{H}$.
- Also when $\mathcal{H}$ is infinite-dimensional and Y is a normal operator (in particular, if Y is unitary).
- This result can be applied to show the convergence of the Baker–Campbell–Hausdorff formula
- The convergence domain can be enhanced by applying *preliminary linear transformations*
- Example: interaction picture in quantum mechanics

Preliminary linear transformations

- Given
$$\frac{dU(t)}{dt} = \tilde{H}(t)U(t),$$
where $\tilde{H} \equiv H/(i\hbar)$, H is the Hamiltonian and U corresponds to the evolution operator, suppose $\tilde{H} = \tilde{H}_0 + \varepsilon\tilde{H}_1$, with $\tilde{H}_0$ a solvable Hamiltonian and $\varepsilon \ll 1$ a small perturbation parameter
- Factorize U as
$$U(t) = G(t)U_G(t)G^\dagger(0),$$
where $G(t)$ is a linear transformation (to be defined yet).
- Then U_G obeys the equation
$$U_G'(t) = \tilde{H}_G(t)U_G(t), \quad \tilde{H}_G(t) = G^\dagger(t)\tilde{H}(t)G(t) - G^\dagger(t)G'(t).$$

Preliminary linear transformations

- A common choice:

$$G(t) = \exp\left(\int_0^t \tilde{H}_0(\tau)d\tau\right)$$

so that

$$\tilde{H}_G(t) = \varepsilon \exp\left(-\int_0^t \tilde{H}_0(\tau)d\tau\right) \tilde{H}_1(t) \exp\left(\int_0^t \tilde{H}_0(\tau)d\tau\right).$$

- This corresponds to the *interaction picture*, but other possibilities exist (e.g., adiabatic picture)

Illustrative example: two-level quantum system

- Rosen–Zener model

$$H(t) = E\sigma_3 + V(t)\sigma_1 \equiv \mathbf{a}(t)\cdot\boldsymbol{\sigma}, \qquad V(t) = V_0/\cosh(t/T),$$

with $\mathbf{a} \equiv (V(t), 0, E)$.

- Parameters: $\gamma = \pi V_0 T/\hbar$, $\xi = 2ET/\hbar$; $s \equiv t/T$
- Here $H_0 = E\sigma_3$ and

$$H_I(s) = V(s)(\sigma_1 \cos(\xi s) - \sigma_2 \sin(\xi s))$$

- Eigenvectors $|+\rangle \equiv (1,0)^T$, $|-\rangle \equiv (0,1)^T$ associated to the eigenvalues $\pm E$ of H_0
- Transition probability between eigenstates $|+\rangle$, $|-\rangle$ of H_0:

$$P(t) = |\langle +|U_I(t)|-\rangle|^2$$

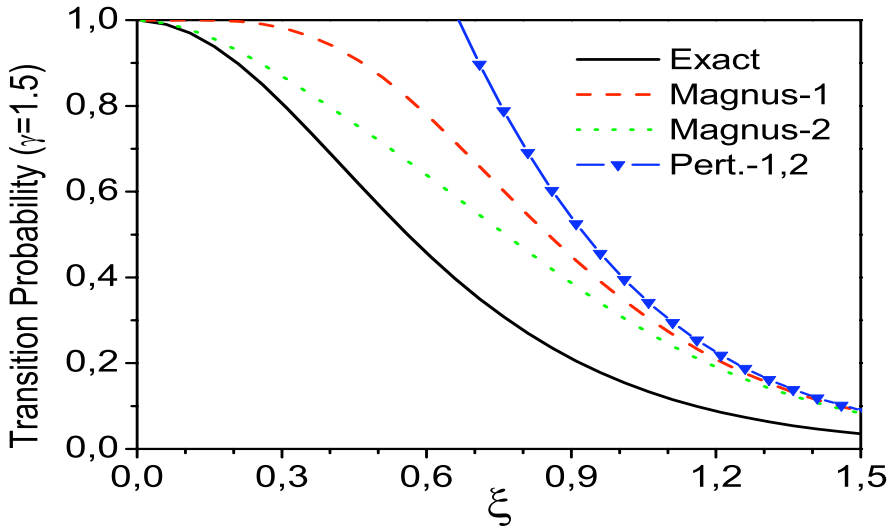
with U_I solution of $U_I' = \tilde{H}_I(t)\, U_I$, $U_I(0) = I$.

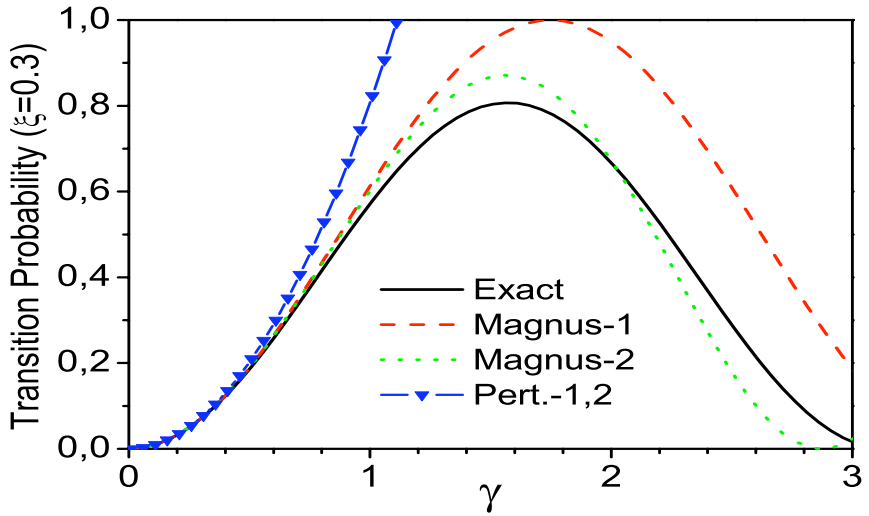
Rosen–Zener model

- The exact result for $P(t)$ is known for the interval $(-\infty, +\infty)$.
- Since

$$\int_{-\infty}^{\infty} \|\tilde{H}_I(t)\|_2 \, dt = (1/\hbar) \int_{-\infty}^{\infty} |V(t)| \, dt = V_0 \pi T/\hbar = \gamma,$$

  the Magnus series converges at least for $\gamma < \pi$.
- Compute Magnus expansion up to Ω_2
- Compare with exact result and perturbation theory
- Compute transition probability
  1. as a function of ξ, with fixed $\gamma = 1.5$
  2. as a function of γ, with fixed $\xi = 0.3$


Transition Probability (γ=1.5)
ξ
Exact
Magnus-1
Magnus-2
Pert.-1,2
0,0
0,2
0,4
0,6
0,8
1,0
0,0
0,3
0,6
0,9
1,2
1,5


Transition Probability (ξ=0.3)
γ
Exact
Magnus-1
Magnus-2
Pert.-1,2
0,0
0,2
0,4
0,6
0,8
1,0
0
1
2
3

Numerical integration?

- Until now we have used the Magnus expansion as a perturbative tool in the treatment of $Y' = A(t)Y$.
- Fairly accurate analytical approximations preserving important qualitative properties
- Several drawbacks, however:
  1. The convergence domain may be relatively small (although it can be improved by using different pictures)
  2. Increasing complex structure of the terms Ω_k: a k-multivariate integral (that has to be approximated) involving $(k-1)$-nested commutators (whose number has to be reduced).
  3. The evaluation of the exponential of a matrix is problematic (especially for high dimensions).
- When the entries of $A(t)$ are complicated functions of time or they are only known for certain values of t, numerical approximation schemes are unavoidable.

Numerical integration?

Question

Is it possible to build numerical integration schemes from the Magnus expansion such that

- the numerical approximations still preserve the main qualitative properties of the exact solution?
- they are computationally efficient and competitive with other standard algorithms?

YES!

Numerical integration?

Question

Is it possible to build numerical integration schemes from the Magnus expansion such that

- the numerical approximations still preserve the main qualitative properties of the exact solution?
- they are computationally efficient and competitive with other standard algorithms?

YES!

Building numerical schemes

Steps in the process:

- Split the time interval $[t_0, t_f]$ into N steps such that the Magnus series converges in each subinterval $[t_{n-1}, t_n]$, $n = 1, \ldots, N$, with $t_N = t_f$. Then

$$Y(t_N) = \prod_{n=1}^{N} \exp(\Omega(t_n, t_{n-1}))\, Y_0,$$

- Truncate the series $\Omega(t_n, t_{n-1})$ at an appropriate order
- Replace the multivariate integrals in the truncated series $\Omega^{[p]} = \sum_{i=1}^{p} \Omega_i$ by conveniently chosen approximations
- Compute the exponential of the matrix $\Omega^{[p]}$

Building numerical schemes

- As a consequence of time-symmetry, $\Omega_{2s+1} = \mathcal{O}(h^{2s+3})$ for $s \geq 1$
- Equivalently, $\Omega^{[2s-2]} = \Omega + \mathcal{O}(h^{2s+1})$ and $\Omega^{[2s-1]} = \Omega + \mathcal{O}(h^{2s+1})$
- For achieving an integration method of order $2s$ ($s > 1$) only terms up to Ω_{2s-2} in the Ω series are required
- Only *even order* methods are considered
- It is possible to approximate all the multivariate integrals appearing in Ω just by evaluating $A(t)$ at the nodes of a univariate quadrature

Scheme of order 4

- Subinterval $[t_n, t_{n+1} = t_n + h]$; $\quad Y_{n+1} \approx Y(t_{n+1})$
- Gauss–Legendre quadrature rule

$$A_1 = A(t_n + (\frac{1}{2} - \frac{\sqrt{3}}{6})h), \qquad A_2 = A(t_n + (\frac{1}{2} + \frac{\sqrt{3}}{6})h)$$

$$\begin{aligned} \Omega^{[4]}(h) &= \frac{h}{2}(A_1 + A_2) - h^2 \frac{\sqrt{3}}{12}[A_1, A_2] \\ Y_{n+1} &= \exp(\Omega^{[4]}(h)) Y_n. \end{aligned}$$

- Alternatively, evaluating A at equispaced points,

$$A_1 = A(t_n), \qquad A_2 = A(t_n + \frac{h}{2}), \qquad A_3 = A(t_n + h)$$

$$\Omega^{[4]}(h) = \frac{h}{6}(A_1 + 4A_2 + A_3) - \frac{h^2}{12}[A_1, A_3].$$

- Two A evaluations and one commutator

Schemes of order 6

$$
\begin{aligned}
C_1 &= [\alpha_1, \alpha_2], \qquad C_2 = -\frac{1}{60}[\alpha_1, 2\alpha_3 + C_1] \\
\Omega^{[6]} &\equiv \alpha_1 + \frac{1}{12}\alpha_3 + \frac{1}{240}[-20\alpha_1 - \alpha_3 + C_1, \alpha_2 + C_2],
\end{aligned}
$$

- Gauss–Legendre collocation points

$$A_1 = A\big(t_n + (\frac{1}{2} - \frac{\sqrt{15}}{10})h\big), \quad A_2 = A\big(t_n + \frac{1}{2}h\big), \quad A_3 = A\big(t_n + (\frac{1}{2} + \frac{\sqrt{15}}{10})h\big)$$

$$\alpha_1 = hA_2, \quad \alpha_2 = \frac{\sqrt{15}h}{3}(A_3 - A_1), \quad \alpha_3 = \frac{10h}{3}(A_3 - 2A_2 + A_1)$$

and finally $Y_{n+1} = \exp(\Omega^{[6]})Y_n$

- Three A evaluations and three commutators

Remarks

- It is also possible to express $\Omega^{[4]}$, $\Omega^{[6]}$ in terms of *univariate integrals*
- 8th-order Magnus methods with only 6 commutators
- Variable step size techniques can be easily implemented
- Next we illustrate these methods again on the Rosen–Zener model in the interaction picture $U_I' = \tilde{H}_I(t) U_I$, and

$$\tilde{H}_I(t) = -iV(s)\big(\sigma_1 \cos(\xi s) - \sigma_2 \sin(\xi s)\big) \equiv -i\,\mathbf{b}(s)\cdot\boldsymbol{\sigma}.$$

Here $V(s) = V_0/\cosh(s)$, $\xi = \omega T$ and $s = t/T$.

Remarks

- It is also possible to express $\Omega^{[4]}$, $\Omega^{[6]}$ in terms of *univariate integrals*
- 8th-order Magnus methods with only 6 commutators
- Variable step size techniques can be easily implemented
- Next we illustrate these methods again on the Rosen–Zener model in the interaction picture $U_I' = \tilde{H}_I(t) U_I$, and

$$\tilde{H}_I(t) = -iV(s)\big(\sigma_1 \cos(\xi s) - \sigma_2 \sin(\xi s)\big) \equiv -i\,\mathbf{b}(s)\cdot\boldsymbol{\sigma}.$$

Here $V(s) = V_0/\cosh(s)$, $\xi = \omega T$ and $s = t/T$.

Numerical illustration

- Initial condition $|+\rangle \equiv (1,0)^T$ at $t = -\infty$
- Compute the transition probability to the state $|-\rangle \equiv (0,1)^T$ at $t = +\infty$
- In practice, $s_0 = -25$ and $s_f = 25$. Then, we determine $(U_I)_{12}(s_f, s_0)$.
- We take a fixed time step h such that the whole numerical integration in $s \in [s_0, s_f]$ is carried out with 50 evaluations of the vector $\mathbf{b}(s)$ for all methods.
- *Similar computational cost*.

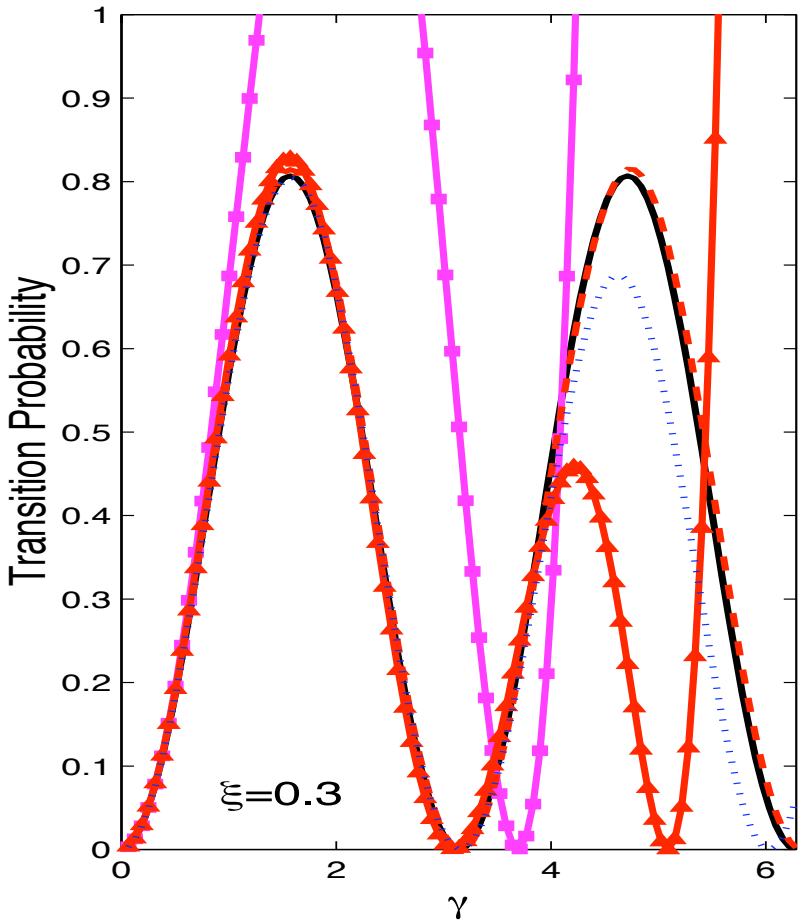
Numerical integrators

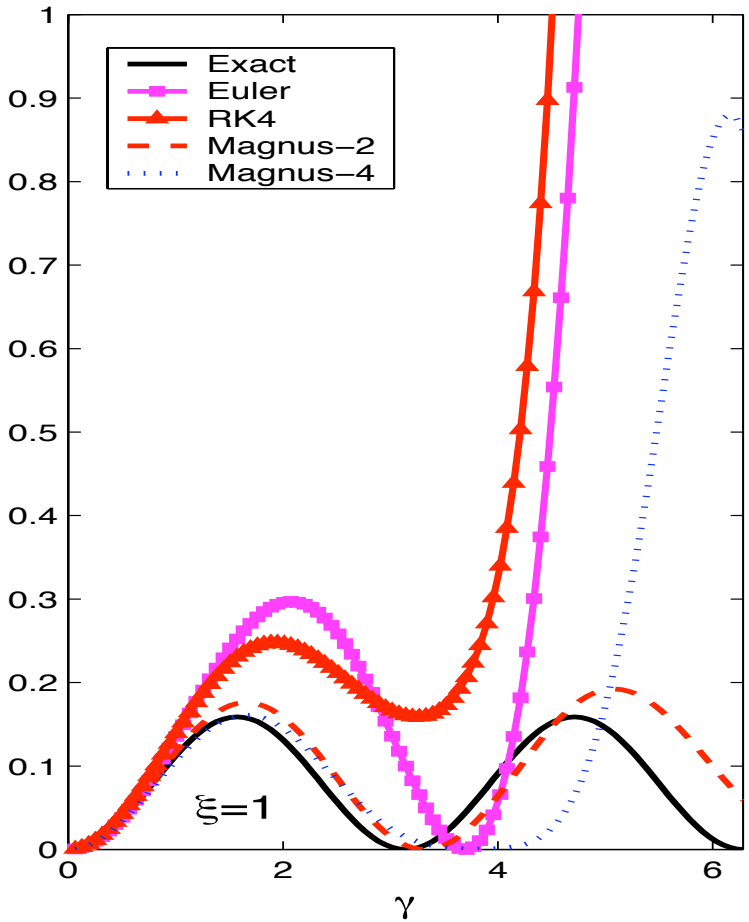
- **Explicit first-order Euler** (E1): $Y_{n+1} = Y_n + hA(t_n)Y_n$ with $t_{n+1} = t_n + h$ and $h = 1$
- **Explicit fourth-order Runge–Kutta** (RK4), with $h = 2$
- **Second-order Magnus** (M2): midpoint rule with $h = 1$

$$Y_{n+1} = \exp\left(-ih\,\mathbf{b}_n \cdot \boldsymbol{\sigma}\right)$$

  with $\mathbf{b}_n \equiv \mathbf{b}(t_n + h/2)$
- **Fourth-order Magnus** (M4) with $h = 2$ and Gauss–Legendre points

We choose $\xi = 0.3$ and $\xi = 1$, and each numerical integration is carried out for different values of γ in the range $\gamma \in [0, 2\pi]$


Transition Probability
ξ=0.3
γ


Exact
Euler
RK4
Magnus–2
Magnus–4
ξ=1
γ

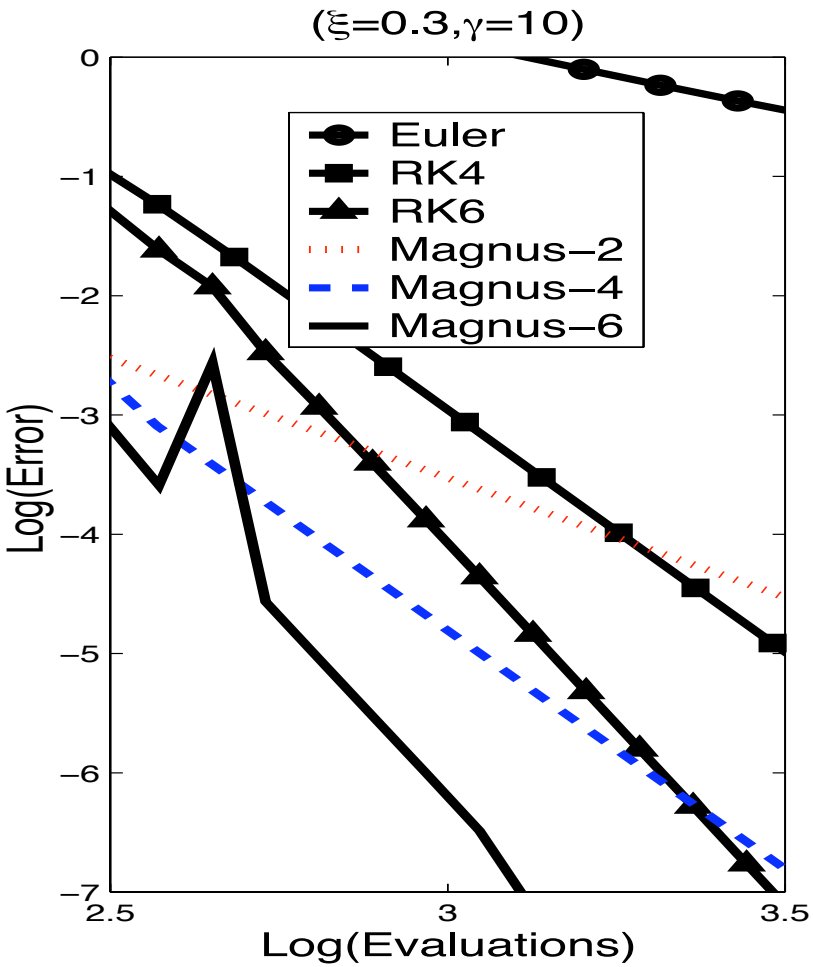
Comments

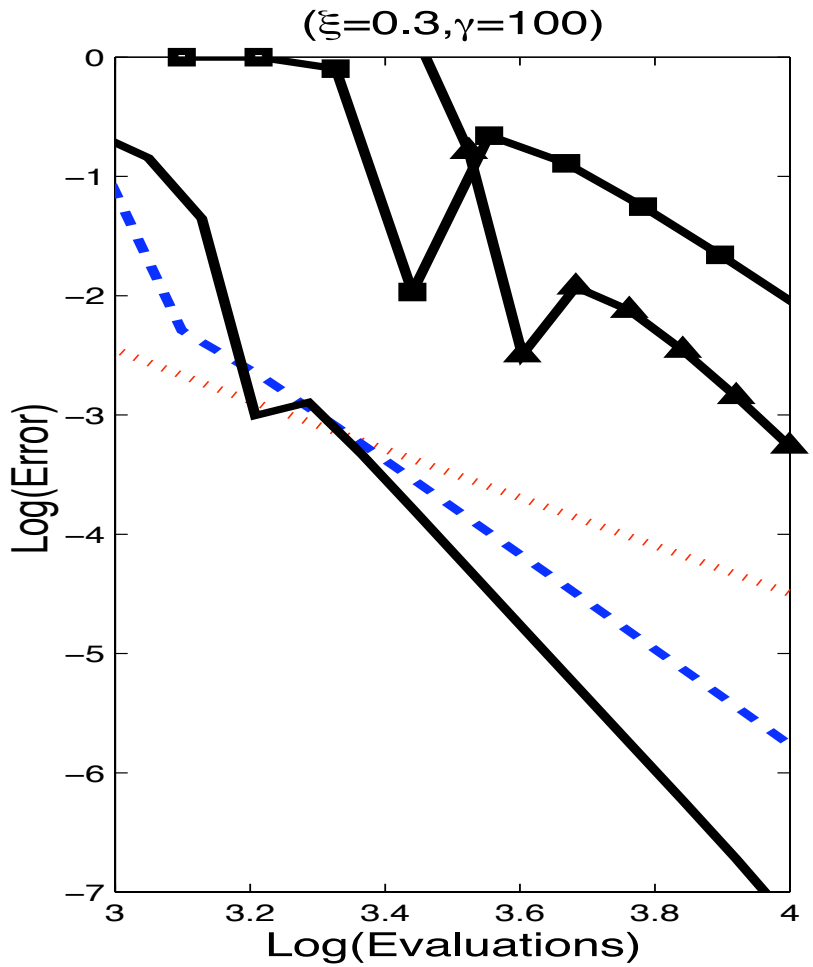
- The performance of the methods deteriorates as γ increases
- Qualitative behavior similar as that exhibited by the analytical approximations: Euler and RK4 do not preserve unitarity (as standard perturbation theory)
- For sufficiently small values of γ (i.e., in the convergence domain) M4 improves the result achieved by M2
- For large values of γ A higher order method does not necessarily lead to a better approximation.

What about efficiency?

- To increase the accuracy, one can always take a smaller h, but then the number of evaluations of $A(t)$ increases, and so does the computational cost.
- Efficiency:
  - better accuracy with the *same* computational cost
  - same accuracy with *less* computational cost
- A good perspective of the overall performance of a given numerical integrator is provided by the *efficiency diagram*
- Error as a function of the total number of matrix evaluations (numerical integration with different time steps), in a double logarithmic scale.
- The slope of the curves corresponds in the limit of very small time steps, to the order of accuracy

Efficiency diagrams (Rosen–Zener)





Matrix exponential

- The previous example requires the computation of the exponential of a 2×2 matrix, for which a closed formula exists.
- How to proceed when the dimension n is higher?
- In that case, the computational cost due to the matrix exponential play an important role
- Several techniques: scaling and squaring with Padé approximation, Chebyshev method, Krylov space methods, splitting, etc.
- What about the efficiency of Magnus then?

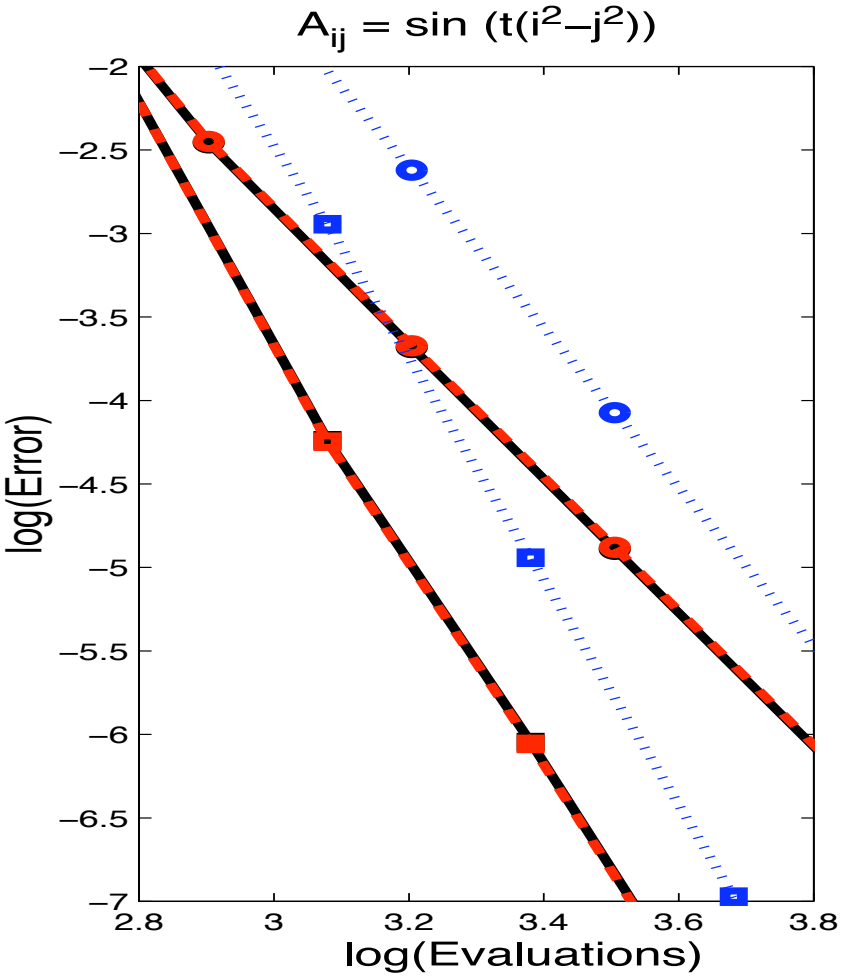
Additional numerical examples

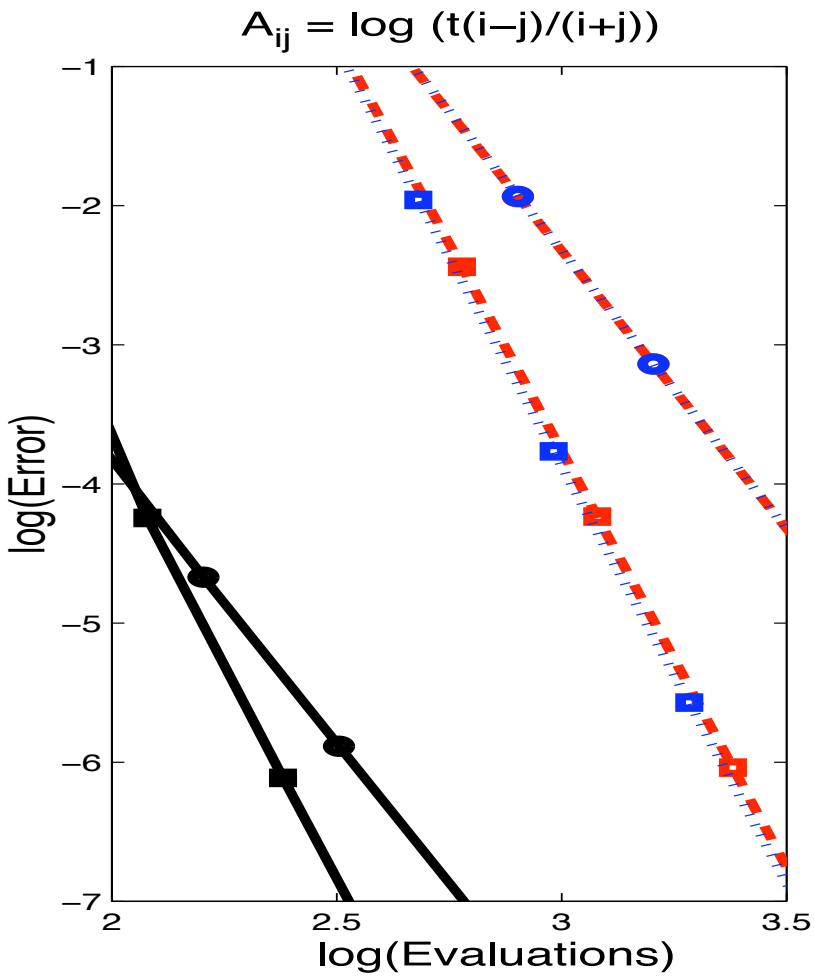
- A couple of skew-symmetric matrices $A(t)$ and $Y(0) = I$, so that the solution $Y(t)$ of $Y' = A(t)Y$ is orthogonal for all t:

$$\begin{aligned} \text{(a)} \quad A_{ij} &= \sin\left(t(j^2 - i^2)\right) \qquad 1 \le i < j \le N \\ \text{(b)} \quad A_{ij} &= \log\left(1 + t\,\frac{j-i}{j+i}\right) \end{aligned}$$

  with $N = 10$

- $Y(t)$ oscillates with time, mainly due to the time-dependence of $A(t)$ (first) or the norm of the eigenvalues (second)
- Integration carried out in $t \in [0, 10]$ and the error is computed at $t_{\mathrm{f}} = 10$
- Compare M4, M6 with RK4, RK6


$A_{ij} = \sin(t(i^2-j^2))$
log(Error)
log(Evaluations)
−2
−2.5
−3
−3.5
−4
−4.5
−5
−5.5
−6
−6.5
−7
2.8
3
3.2
3.4
3.6
3.8


$A_{ij} = \log(t(i-j)/(i+j))$
log(Error)
log(Evaluations)
−1
−2
−3
−4
−5
−6
−7
2
2.5
3
3.5

Back to the Schrödinger equation

- At the beginning, after a space discretization, we ended up with

$$i\frac{d\psi}{dt}(t) = H(t)\psi(t), \qquad \psi(0) = \psi_0$$

  where $\psi(t)$ represents a complex vector with d components which approximates the (continuous) wave function
- We can use numerical methods based on the Magnus expansion
- M2 (exponential midpoint rule):

$$\psi_{n+1} = \exp(-i\Delta t\, H(t_{n+1/2}))\,\psi_n.$$

- If higher order approximations are considered, the accuracy can be enhanced

Back to the Schrödinger equation

- BEWARE!: the theory of Magnus-type methods has been deduced when $h\|H(t)\| \longrightarrow 0$ and is obtained by studying the remainder of the truncated Magnus series
- In the Schrödinger equation, one has discretizations of unbounded operators!
- It turns out that M4 works extremely well even with h for which the corresponding $h\|H(t)\|$ is large (Hochbruck & Lubich)
- In particular, it retains fourth order of accuracy in h *independently of the norm* of $H(t)$ when $H(t) = T + V(t)$
- This is so *even when there is no guarantee that the Magnus series converges at all*

Issues not analyzed here

- Generalizations:
  1. Periodic problems: $A(t+T) = A(t)$ Floquet–Magnus expansion
  2. Nonlinear matrix equations: $Y' = A(t, Y)Y$
  3. Isospectral flows: $Y' = [A(t, Y), Y]$
  4. *General nonlinear equations*
- Numerical schemes based on Magnus *without commutators*
- How to use the Magnus expansion to get new splitting methods for general time-dependent problems: S. Blanes's talk

Basic references

- W. Magnus, On the exponential solution of differential equations for a linear operator, *Commun. Pure Appl. Math.* **7** (1954), 649-673.
- A. Iserles, S.P. Nørsett, On the solution of linear differential equations in Lie groups, *Phil. Trans. R. Soc. A* **357** (1999), 983-1019.
- S. Blanes, F. Casas, J.A. Oteo, J. Ros, The Magnus expansion and some of its applications, *Phys. Rep.* **470** (2009), 151-238.