On Magnus integrators for time-dependent Schrödinger equations

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Outline

• Time dependent Schrödinger equations

\[ i \frac{d\psi}{dt} = H(t)\psi, \quad \psi(t_0) = \psi_0 \]

• Magnus integrators

• Error bounds for Magnus integrators of order 2 and 4

• Sketch of general procedure for deriving these bounds

• Numerical experiment
Short course on Magnus integrators

\[ y' = A(t)y, \quad y(0) = y_0 \]

Magnus approach '54: determine \( \Omega(t) \) such that

\[ y(t) = \exp(\Omega(t))y_0 \]

solution of \( y' = A(t)y \)

\( \Omega(t) = tA \) for \( A(t) \equiv A \)

Differentiate

\[ y'(t) = \text{dexp}_{\Omega(t)}(\Omega'(t))y(t), \]

where

\[ \text{dexp}_\Omega(B) = \varphi(\text{ad}_\Omega)(B) = \sum_{k \geq 0} \frac{1}{(k + 1)!} \text{ad}_\Omega^k(B), \quad \varphi(z) = \frac{e^z - 1}{z} \]

and \( \text{ad}_\Omega(B) = [\Omega, B] = \Omega B - B\Omega. \)

Obtain \( \Omega \) as solution of

\[ A(t) = \text{dexp}_{\Omega(t)}(\Omega'(t)), \quad \Omega(0) = 0 \]
Magnus integrators II

If $\|\Omega(t)\| < \pi$, then $\text{dexp}_{\Omega(t)}$ is invertible

$$\text{dexp}_{\Omega(t)}^{-1}(A(t)) = \sum_{k \geq 0} \frac{\beta_k}{k!} \text{ad}_{\Omega(t)}^k(A(t)), \quad \beta_k \text{ kth Bernoulli number}$$

obtain

$$\Omega'(t) = A(t) - \frac{1}{2} [\Omega(t), A(t)] + \frac{1}{12} [\Omega(t), [\Omega(t), A(t)]] + \ldots$$

integration and Picard iteration yields Magnus expansion

$$\Omega(t) = \int_0^t A(\tau)d\tau - \frac{1}{2} \int_0^t \left[ \int_0^\tau A(\sigma)d\sigma, A(\tau) \right] d\tau$$

$$+ \frac{1}{4} \int_0^t \left[ \int_0^\tau \left[ \int_0^\sigma A(\mu)d\mu, A(\sigma) \right] d\sigma, A(\tau) \right] d\tau$$

$$+ \frac{1}{12} \int_0^t \left[ \int_0^\tau A(\sigma)d\sigma, \left[ \int_0^\tau A(\mu)d\mu, A(\tau) \right] \right] d\tau + \ldots$$
Magnus integrators III

Numerical methods (review: Iserles, Munthe-Kaas, Nørsett, Zanna, '00)

\[ y_{n+1} = \exp(\Omega_n)y_n \quad \Omega_n \approx \Omega(h) \]

Approximation involves

- truncating the Magnus expansion (after \( k \) terms)

\[
k = 1 : \quad \tilde{\Omega}(t) = \int_0^t A(t_n + \tau)d\tau
\]

\[
k = 2 : \quad \tilde{\Omega}(t) = \int_0^t A(t_n + \tau)d\tau - \frac{1}{2} \int_0^t \left[ \int_0^{\tau} A(t_n + \sigma)d\sigma, A(t_n + \tau) \right] d\tau
\]

- approximating integrals by replacing \( A(t) \) by interpolation polynomial \( \hat{A}(t) \) for quadrature nodes \( t_n + c_j h \)
Examples:

\( k = 1, \) exponential midpoint rule

\[
\Omega_n = hA(t_n + h/2).
\]

\( k = 2, \) 2-point Gauß quadrature rule:

\[
\Omega_n = \frac{h}{2}(A_1 + A_2) + \frac{\sqrt{3}h^2}{12}[A_2, A_1], \quad A_j = A(t_n + c_j h),
\]

\( c_j \) nodes of Gauß quadrature rule

\( k = 2, \) method by Blanes, Casas, Ros ’00

\[
\Omega_n = \frac{h}{6}(A(t_n) + 4A(t_{n+1/2}) + A(t_{n+1})) - \frac{h^2}{12}[A(t_n), A(t_{n+1})].
\]
Implementation issues

options for computing $\exp(\Omega)y$:

- splitting methods
- Chebyshev approximation
- Lanczos process
Situation

- Magnus integrators efficient for problems like Schrödinger equations (Tal Ezer, Kosloff, '92; Blanes, Moan, '00)
- error behavior well understood for $\|A(t)\|$ moderate (Iserles, Nørsett, '99; Iserles, Munthe-Kaas, Nørsett, Zanna '00)
- no results for $h \|A(t)\| \gg 1$
Problems for large $h \| A(t) \|$

- $d \exp \Omega$ need not be invertible
- Magnus expansion need not converge
- known results on order of Magnus integrators valid for $h \| A(t) \| \to 0$
  (Iserles, Nørsett, '99)
  - constants involve $\| A(t) \|$
  - obtained by studying remainder of Magnus series

Practice: Magnus integrators work extremely well even for $h \| A(t) \| \gg \pi$

WHY?
General assumptions

\[ A(t) = -iH(t) = -i(U + V(t)) \]

where \( U \) s.p.d., \( V(t) \) hermitian satisfying

\[
\left\| \frac{d^m}{dt^m} V(t) \right\| \leq M_m, \quad m = 0, 1, 2, \ldots
\]

but no bound on \( \|U\| \)!

define

\[ D = U^{1/2} \]
typical situation:

\[ U = -\Delta + I, \quad V \text{ bounded multiplication operator} \]

continuous case: \((Q \text{ cube, periodic boundary conditions})\)

\[ \|Dv\|^2 = \int_Q |\nabla v|^2 dx + \int_Q v^2 dx \]

\(\|Dv\|\) is \(H^1\) Sobolev norm

\(\|Dy(t)\|\) is essentially the kinetic energy of the solution (bounded a priori)

discrete case, minimal grid spacing \(\Delta x\):

\[ \|U\| \sim \Delta x^{-2}, \quad \|D\| \sim \Delta x^{-1} \]
Exponential midpoint rule

**Theorem** (H., Lubich ’02)

If the solution $y$ satisfies the finite energy condition

$$y(t)^* H(t) y(t) \leq K,$$

then the error of exponential midpoint rule is bounded by

$$\|y_n - y(t_n)\| \leq Ch^2 t_n \max_{0 \leq t \leq t_n} \|Dy(t)\|$$

where $C = C(M_m, K)$, $m \leq 2$

Error bound for classical implicit midpoint rule:

$$\|y_n - y(t_n)\| \leq Ch^2 t_n \max_{0 \leq t \leq t_n} \left\| \frac{d^3}{dt^3} y(t) \right\|$$
Fourth order Magnus methods – assumptions

commutator bounds:

for a method of order $p$ containing products of $A(t_n + c_j h)$ with $r$ terms we need

$$\| [A(\tau_k), \ldots, [A(\tau_1), \frac{d^m}{dt^m} V(\tau_0)] \ldots] v \| \leq K \| D^k v \| \quad \left\{ \begin{array}{l} 0 \leq m \leq p, \\ k + 1 \leq rp. \end{array} \right.$$ 

(easy for spatially cont. case,
 discrete case: generalization of results of Jahnke, Lubich, '00)

in our examples: $p = 4, r = 2$
**Theorem** (H., Lubich ’02)

If the commutator bounds hold for \( p = 4 \) and \( r = 2 \), then error of fourth order Magnus methods is bounded by

\[
\|y_n - y(t_n)\| \leq Ch^4 t_n \max_{0 \leq t \leq t_n} \|D^3y(t)\|
\]

for time steps \( h \|D\| \leq c \)

with \( C = C(M_m, K, c), m \leq 4 \).

**Remarks:**

- explicit integrators require \( h\|D\|^2 \leq c \) for stability,
- error bounds for implicit integrators require smallness of \( h\|D\|^2 \) for oscillatory problems
General procedure for deriving error bounds

(complete proofs for exponential midpoint rule and fourth order methods)

- cannot use derivation, in particular not $A = d\exp_\Omega(\Omega')$
- cannot use Taylor expansion of solution
1. Error resulting from truncating the Magnus expansion:

Motivation: Magnus approach starts from

\[ y(t) = \exp(\Omega(t))y_0, \quad \Omega \text{ skew} \]

truncation yields

\[ \tilde{y}(t) = \exp(\tilde{\Omega}(t))y_0, \quad \tilde{\Omega} \text{ skew} \]

differentiate: \( \tilde{y}(t) \) is solution of perturbed problem

\[ \tilde{y}'(t) = \tilde{A}(t)\tilde{y}(t) \quad \text{with} \quad \tilde{A}(t) = \text{dexp}_{\tilde{\Omega}(t)}(\tilde{\Omega}'(t)) \]

with initial value \( \tilde{y}(0) = y_0 \), \( \tilde{A}(t) \) skew hermitian

**Lemma** \[ \| \tilde{y}(t) - y(t) \| \leq \int_0^t \| E(\tau)y(\tau) \| d\tau, \quad E = \tilde{A} - A \]
2. Remainder of $\text{dexp}$ series

recall:

$$\text{dexp}_\Omega(B) = \varphi(\text{ad}_\Omega)(B)$$

truncate $\varphi$ appropriately

$$\varphi(z) = \frac{e^z - 1}{z} = 1 + \frac{1}{2}z + \ldots + \frac{1}{(p-1)!} z^{p-2} + \frac{1}{p!} z^{p-1} r_p(z),$$

obtain remainder of truncated $\text{dexp}_\Omega$ series

$$\text{dexp}_\Omega(B) = B + \frac{1}{2} [\Omega, B] + \ldots + \frac{1}{(p-1)!} \text{ad}_\Omega^{p-2}(B) + \frac{1}{p!} r_p(\text{ad}_\Omega)\left(\text{ad}_\Omega^{p-1}(B)\right)$$

we need a bound of type

$$\| r_p(\text{ad}_{\tilde{\Omega}(t)})\left(\text{ad}_{\tilde{\Omega}(t)}^{p-1}(\tilde{\Omega}'(t))\right) v\| \leq Ch^p \| D^{p-1}v\|, \quad 0 \leq t \leq h,$$

requires $h\|D\| \leq c$ for $p = 4$, no restriction on $h$ for $p = 2$
Bound on \( Ev = (\tilde{A} - A)v \)

exponential midpoint rule \((p = 2)\):

\[
\tilde{\Omega}(t) = \int_0^t A(t_n + \tau) d\tau
\]

and

\[
\tilde{A}(t) = \text{dexp}_{\tilde{\Omega}(t)}(\tilde{\Omega}'(t)) = A(t) + \frac{1}{2} r_2(\text{ad}_{\tilde{\Omega}(t)})(\text{ad}_{\tilde{\Omega}(t)}(\tilde{\Omega}'(t))) =: A(t) + E_2(t)
\]

Lemma

For \( p = 2, 4 \): \( \| E_p(t)y(t) \| \leq Ch^p\| D^{p-1}y(t) \|, \quad 0 \leq t \leq h \)

where for \( p = 4 \), \( h\| D \| \leq c \)
3. Error resulting from approximating the integrals

nth step: write $\tilde{\Omega}_n = \tilde{\Omega}(h)$ for truncated Magnus series

quadrature: use $\Omega_n$ instead of $\tilde{\Omega}_n$

e.g., for the midpoint rule

$$
\tilde{\Omega}_n = \int_0^h A(t_n + \tau) d\tau \approx hA(t_{n+1/2}) =: \Omega_n
$$

since $\|A''(t)\| = \|V''(t)\| \leq M_2$, we have $\|\tilde{\Omega}_n - \Omega_n\| \leq \frac{1}{24} M_2 h^3$

**Lemma**

$$
\| (\tilde{\Omega}_n - \Omega_n) v \| \leq Ch^{p+1} \| D^{r-1} v \|
$$

($p = 2, r = 1$, proof more difficult for $p = 4, r = 2$)

**Lemma**

$$
\| \exp(\tilde{\Omega}_n) v - \exp(\Omega_n) v \| \leq Ch^{p+1} \| D^{r-1} v \|
$$

(obvious for $r = 1$)
4. Putting all steps together

define local error

\[
\epsilon_n = y(t_{n+1}) - \exp(\Omega_n)y(t_n)
\]

\[
= y(t_{n+1}) - \exp(\tilde{\Omega}_n)y(t_n) + \exp(\tilde{\Omega}_n)y(t_n) - \exp(\Omega_n)y(t_n)
\]

\[
= y(t_{n+1}) - \tilde{y}(t_{n+1}) + \exp(\tilde{\Omega}_n)y(t_n) - \exp(\Omega_n)y(t_n)
\]

by Steps 1–3

\[
\|\epsilon_n\| \leq \int_{t_n}^{t_{n+1}} \|E_p(\tau)y(\tau)\|d\tau + Ch^{p+1}\|D^{r-1}y(t_n)\|
\]

\[
\leq Ch^{p+1}\max_{t_n \leq t \leq t_{n+1}} \|D^{p-1}y(t)\|
\]

error recursion for global error \(e_n = y_n - y(t_n)\):

\[
e_{n+1} = \exp(\Omega_n)e_n + \epsilon_n
\]

yields

\[
\|e_n\| \leq Ct_n h^p \max_{0 \leq t \leq t_n} \|D^{p-1}y(t)\|
\]
Numerical experiment

\[ i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \Delta \psi + b(x, t) \psi, \quad x = (x_1, \ldots, x_d) \in \mathbb{R}^d, \quad t > 0 \]

discretized such that \( h\|D\| \approx 3.5 \) (\( N = 32, \ldots, 2048 \) Fourier modes)
Summary

Known in practice: Magnus methods work well for time-dependent Schrödinger equations here: theoretical explanation for this behavior, in particular

- presented optimal-order error estimates for problems where $h\|H(t)\|$ is large
- developed new mechanisms which lead to such bounds