

The Magnus expansion in the adiabatic picture

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Outline

- 1 Adiabatic evolution of linear problems
- 2 Magnus expansion: direct approach
- 3 Magnus expansion: adiabatic picture
- 4 Analysis of two examples
 - Classical simple harmonic oscillator
 - Time-dependent two-state quantum system
- 5 Conclusions

Formulation of the Problem

- Linear systems of the form

$$\frac{dU}{d\tau} = \frac{1}{\varepsilon} S(\tau)U, \quad U(\tau_0) = I \quad (1)$$

with the parameter $0 < \varepsilon \ll 1$ and $S(\tau)$, $U(\tau)$ $n \times n$ matrices.

- How they appear?
- Typically, when $S(t)$ depends smoothly on time through the variable $\tau = t/T$, where T determines the time scale and $T \rightarrow \infty$
- Then one has $\frac{dU}{dt} = S(\varepsilon t)U$, $\varepsilon \equiv 1/T \ll 1$ or equivalently, eq. (1) with $\tau \equiv \varepsilon t$.

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Formulation of the Problem

- Two different time-scales in the problem
- The parameter ε controls the separation of time-scales: the smaller ε , the slower the variation of $S(\varepsilon t)$ on the a priori fixed **fast** time-scale t .
- The time variable $\tau = \varepsilon t$ on which S varies is called the **slow** time-scale

Some examples

- Classical Mechanics. Time-dependent harmonic oscillator, with

$$H(q, p, t) = \frac{1}{2}(p^2 + \omega^2(\varepsilon t)q^2)$$

- The ‘action’ $J(\tau) \equiv H(\tau)/\omega(\tau)$ is an **adiabatic invariant**: it remains approximately constant during a time interval of order $1/\varepsilon$.
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- Quantum Mechanics. Time-dependent Schrödinger equation in the **adiabatic** (infinitely slow) limit

$$i\hbar \frac{d\psi}{d\tau} = \frac{1}{\varepsilon} H(\tau)\psi, \quad (2)$$

- **Quantum Adiabatic Theorem** (Born, Fock): absolute values of the coefficients in the eigenbasis representation of ψ are adiabatic invariants as $\varepsilon \rightarrow 0$.

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Several theoretical issues

- Existence of geometric contributions: Berry's phase (QM), Hannay's angle (CM)
- (Exponentially small) transition probabilities (QM)
- J : '...many of the difficulties in determining the degree to which an adiabatic invariant is invariant have not yet been overcome to this day' (Sagdeev, Usikov, Zaslavsky)
- Computation of $\delta J = J(t) - J(t_0)$ for a time interval $\gg 1/\varepsilon$
- Computation of $\Delta J = J(+\infty) - J(-\infty)$: asymptotic analysis, etc. when $\varepsilon \rightarrow 0$ (Littlewood, Meyer, J.B. Keller, Wasow, Kruskal, Joye, Boutet de Monvel, ...)

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Several theoretical issues

- Study of the evolution when ε is not so small (near-adiabatic regime)
- Construction of numerical integration schemes in this setting (T. Jahnke, C. Lubich, K. Lorenz): **adiabatic integrators**
- Our approach: Magnus expansion applied to

$$\frac{dU}{d\tau} = \frac{1}{\varepsilon} S(\tau)U, \quad U(\tau_0) = I$$

in the **adiabatic picture**.

- Based on: Klarsfeld, Oteo (1992); C. (1992); C., Oteo, Ros (1994) **and** some new results on convergence and quadratures

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Magnus expansion

Given

$$\frac{dY}{dt} = A(t)Y, \quad Y(0) = I$$

then

$$Y(t) = e^{\Omega(t)}, \quad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t)$$

- $\Omega_k(t)$: sum of k -fold integrals of $k - 1$ nested commutators
- Explicit expressions for all Ω_k
- Existence of several recurrences

Magnus expansion

First terms of the expansion ($A_i \equiv A(t_i)$):

$$\Omega_1 = \int_0^t A(t_1) dt_1$$

$$\Omega_2 = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2]$$

$$\Omega_3 = \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1, [A_2, A_3]] + [A_3, [A_2, A_1]])$$

Convergence of the Magnus expansion

Theorem

The Magnus series $\Omega(t) = \sum_{k=1}^{\infty} \Omega_k$ converges for $0 \leq t < T$ such that

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

and the sum $\Omega(t)$ satisfies $\exp \Omega(t) = Y(t)$

- Moan, Niesen (2006): valid for a $n \times n$ real matrix $A(t)$
- C. (2007): $A(t)$ any bounded operator in a Hilbert space

Adiabatic case

For the problem

$$\frac{dU}{d\tau} = \frac{1}{\varepsilon} S(\tau)U, \quad U(\tau_0) = I$$

with $0 < \varepsilon \ll 1$, the above expansion is meaningless, since

- $\Omega(\tau) = \sum_{k=1}^{\infty} \frac{1}{\varepsilon^k} \Omega_k(t)$
- the convergence domain is too restrictive:

$$\int_0^T \|S(\tau)\| d\tau < \varepsilon \pi$$

(In fact, the greater ε , the better the convergence of Magnus expansion)

The formalism

Suppose we have

$$\dot{U} \equiv \frac{dU}{d\tau} = \frac{1}{\varepsilon} S(\tau) U, \quad U(0) = I,$$

such that $S(\tau)$ can be instantaneously diagonalized:

$$U_0^{-1}(\tau) S(\tau) U_0(\tau) = \Lambda(\tau) = \text{diag}(\lambda_1(\tau), \lambda_2(\tau), \dots)$$

with

$$|\lambda_k(\tau) - \lambda_l(\tau)| \geq \delta_m > 0, \quad k \neq l$$

'Adiabatic' picture: change of coordinates to the basis defined by the eigenvectors of S

The formalism

Then

$$U_1(\tau) = U_0^{-1}(\tau)U(\tau)U_0(0) \quad U(\tau) = U_0(\tau)U_1(\tau)U_0^{-1}(0)$$

with

$$\dot{U}_1 = S_1(\tau)U_1, \quad S_1 = \frac{1}{\varepsilon}\Lambda(\tau) - U_0^{-1}\dot{U}_0$$

Now we split $S_1 = (S_1)_d + (S_1)_{nd}$:

$$(S_1)_d = \frac{1}{\varepsilon}\Lambda - (U_0^{-1}\dot{U}_0)_d, \quad (S_1)_{nd} = -(U_0^{-1}\dot{U}_0)_{nd}$$

diagonal + non-diagonal part

The formalism

Next, **'interaction' picture**: $U_1(\tau) = U_d(\tau)U_2(\tau)$, with

$$U_d(\tau) = \exp \int_0^\tau (\mathcal{S}_1)_d(\tau_1) d\tau_1$$

Thus

$$\dot{U}_2 = \mathcal{S}_2(\tau)U_2, \quad U_2(0) = I$$

with

$$\mathcal{S}_2(\tau) = U_d^{-1}(\tau)(\mathcal{S}_1)_{nd}(\tau)U_d(\tau) = -U_d^{-1}(\tau)(U_0^{-1}\dot{U}_0)_{nd}(\tau)U_d(\tau)$$

The formalism

Naive approach:

$$U_2(\tau) = I + \int_0^\tau S_2(\tau_1) U_2(\tau_1) d\tau_1 \quad (3)$$

- $S_2(\tau)$ is non-diagonal and, if the eigenvalues of S are purely imaginary, its elements contain terms of the form $\exp(\frac{i}{\varepsilon}g(\tau))$ (**highly oscillatory**)
- When $\varepsilon \rightarrow 0$, the integral in (3) vanishes
- In QM: *adiabatic theorem*
- Computing $U_2(\tau)$ is all we need to obtain the evolution of U

Finally, Magnus again

One possible approach: apply Magnus expansion to

$$\dot{U}_2 = \mathcal{S}_2(\tau)U_2, \quad U_2(0) = I$$

In this way,

$$U(\tau) = U_0(\tau)U_d(\tau) e^{\Omega(\tau)} U_0^{-1}(0)$$

- Preservation of qualitative properties when the series is truncated. In QM, the scheme is **unitary**.
- More favourable convergence properties. If U_0 , U_d are unitary,

$$\int_0^\tau \|\mathcal{S}_2(\tau_1)\| d\tau_1 \leq \int_0^\tau \|\dot{U}_0(\tau)\| d\tau_1 < \pi$$

Remarks

- In $(S_1)_d$ (and therefore in U_d) there is a term coming from $U_0^{-1} \dot{U}_0$
- This is a **geometric contribution**, with consequences in probability transitions, adiabatic invariant, etc.
- The Magnus expansion in the adiabatic picture has important differences with respect to the direct approach, both in the convergence domain and in the dependence of each term Ω_k

Simple harmonic oscillator

$$\ddot{q} = -\omega^2(\varepsilon t)q$$

In this case,

$$S(\tau) = \begin{pmatrix} 0 & 1 \\ -\omega^2 & 0 \end{pmatrix}$$

with eigenvalues $\pm i\omega$. Then

$$S_2(\tau) = \begin{pmatrix} 0 & -\frac{i}{\omega(\tau_0)}f(\tau) \\ i\omega(\tau_0)f^*(\tau) & 0 \end{pmatrix}$$

where $f(\tau) \equiv \frac{\dot{\omega}}{2\omega} \exp\left(-2i\varepsilon^{-1} \int_{\tau_0}^{\tau} \omega(\tau_1) d\tau_1\right)$

Classical simple harmonic oscillator

Convergence domain for the Magnus expansion:

$$\int_{\tau_0}^{\tau} \|\mathbf{S}_2(\tau_1)\|_2 d\tau_1 = \frac{1}{2} m_0 \int_{\tau_0}^{\tau} |(\dot{\omega}/\omega)| d\tau_1 < \pi$$

with $m_0 \equiv \max\{|\omega(\tau_0)|, |\omega(\tau_0)|^{-1}\}$

Wasow example

$$\omega^2(\tau) = 1 + (1 + 2e^{-\tau})^{-1}$$

- $\omega(\tau) > 0$ and $\frac{\dot{\omega}}{\omega} > 0$ for all real τ
- Limits at infinity: $\omega_- = 1$, $\omega_+ = \sqrt{2}$
- Derivative $\omega^{(n)} = \mathcal{O}(e^{\pm\tau})$ as $\tau \rightarrow \mp\infty$

If $\tau_0 \rightarrow -\infty$, then $\omega(\tau_0) \approx 1$ and $m_0 = 1$,

$$\int_{\tau_0}^{\tau} \|\mathbf{S}_2(\tau_1)\|_2 d\tau_1 = \frac{1}{2} \log \omega(\tau) < \pi$$

or $\omega(\tau) < e^{2\pi} \approx 535.492$ and thus **convergence for all τ**

Simple harmonic oscillator

- In general, if $\omega(\pm\infty) = \omega_{\pm}$ and $\omega(\varepsilon t) > \text{const} > 0$, there exist the limit values $J(+\infty)$ and $J(-\infty)$ of the adiabatic invariant and we can compute

$$\Delta J = J(+\infty) - J(-\infty)$$

- If ω is analytic, then ΔJ is exponentially small in $1/\varepsilon$
- One can compute the leading term in the asymptotic expansion of ΔJ when $\varepsilon \rightarrow 0$
- With Magnus, we can compute $\delta J = J(\tau) - J(\tau_0)$ for any time and thus analyze non-adiabatic effects

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Simple harmonic oscillator

- Let $\xi(\tau) = (q(\tau), p(\tau))^T$ such that $\dot{\xi}(\tau) = U(\tau)\xi(\tau)$.
- Let $\xi_U(\tau) = (q_U(\tau), p_U(\tau))^T$ such that $\dot{\xi}_U(\tau) = U_0^{-1}\xi_U(\tau)$
- Then $J(\tau) = -iq_U(\tau)p_U(\tau)$ and **Magnus-1** applied to S_2 gives δJ in terms of only one integral
- Taking $\tau_0 \rightarrow -\infty$ and $\tau \rightarrow +\infty$,

$$\Delta J = \frac{\sinh 2|\mathcal{K}|}{2|\mathcal{K}|} \left(\omega_- \mathcal{K}^* q_U^2(-\infty) - \frac{1}{\omega_-} \mathcal{K} p_U^2(-\infty) \right) - 2iq_U(-\infty)p_U(-\infty) \sinh^2 |\mathcal{K}|$$

Simple harmonic oscillator

$$\mathcal{K} = \int_{-\infty}^{+\infty} d\tau \frac{\dot{\omega}(\tau)}{2\omega(\tau)} \exp\left(-\frac{2i}{\varepsilon} \Theta(\tau)\right) \quad \Theta(\tau) = \int_0^\tau \omega(\tau_1) d\tau_1$$

- \mathcal{K} also appears in the study of the above barrier 1-d scattering problem
- Asymptotic treatment of \mathcal{K} assuming that $\omega(\tau)$ is analytic on a neighborhood of the real τ -axis and

$$\omega(\tau) = \omega_0(\tau - \tau_c)^{\nu/2} \left(1 + \sum_{j=1}^{\infty} \omega_j(\tau - \tau_c)^j \right), \quad \nu \in \mathbb{R}, \omega_0 \neq 0$$

in the vicinity of 'transition points' τ_c (roots, isolated singular points, branch points).

Simple harmonic oscillator

- If $\zeta_c = \Theta(\tau_c)$, $\text{Im } \zeta_c = -m$, then

$$\Delta J \simeq \frac{i\pi\nu}{\nu + 2} e^{-2m/\varepsilon} (\omega_- \varphi q_U^2(-\infty) + \omega_-^{-1} \varphi^* p_U^2(-\infty))$$

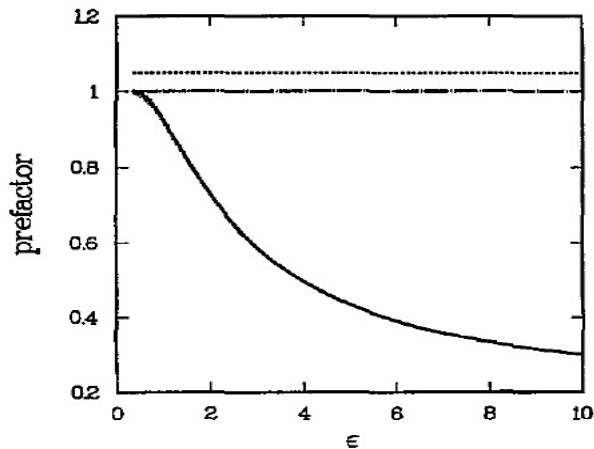
where $\varphi = \exp((2i/\varepsilon)\text{Re } \zeta_c)$.

- Wasow example: $\tau_c = -i\pi$, $\nu = 1$, $\text{Im } \zeta_c = -\pi$, and

$$|\Delta J| \simeq P e^{-2\pi/\varepsilon} + o(e^{-2\pi/\varepsilon})$$

with $P \equiv \frac{\pi}{3} |\varphi q_U^2(-\infty) + \varphi^* p_U^2(-\infty)|$

Prefactor $e^{2\pi/\varepsilon} |\Delta J|$ vs. ε



Prototypical problem (Two-level system)

$$i\frac{d\psi}{d\tau} = \frac{1}{\varepsilon}H(\tau)\psi, \quad (4)$$

and the Hamiltonian H is the real-symmetric 2×2 -matrix

$$H(\tau) = E(\tau) \begin{pmatrix} \cos \theta(\tau) & \sin \theta(\tau) \\ \sin \theta(\tau) & -\cos \theta(\tau) \end{pmatrix}$$

with eigenvalues $\pm E(\tau)$. Assume that

- $2E(\tau) \geq \text{const} > 0$ for all real τ
- $\theta(\tau)$ is asymptotically constant as $\tau \rightarrow \pm\infty$.

Two-level quantum system

In this case $S(\tau) = -iH(\tau)$,

$$U_0(\tau) = \begin{pmatrix} \cos \frac{\theta}{2} & \sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & -\cos \frac{\theta}{2} \end{pmatrix} = U_0^{-1}(\tau),$$

$$U_d(\tau) = \begin{pmatrix} e^{-iw(\tau)/\varepsilon} & 0 \\ 0 & e^{iw(\tau)/\varepsilon} \end{pmatrix}$$

with $w(\tau) \equiv \int_{\tau_0}^{\tau} E(\tau_1) d\tau_1$

Convergence condition

$$\dot{U}_2 = S_2(\tau)U_2$$

$$S_2(\tau) = \frac{\dot{\theta}}{2} \begin{pmatrix} 0 & -e^{2i\omega(\tau)/\varepsilon} \\ e^{-2i\omega(\tau)/\varepsilon} & 0 \end{pmatrix}$$

so that

$$\int_0^\tau \|S_2(\tau_1)\|_2 d\tau_1 = \frac{1}{2}|\theta(\tau) - \theta(\tau_0)|$$

but $|\theta(\tau) - \theta(\tau_0)| < 2\pi$ always. Therefore, **Magnus expansion is always convergent**

Velocity of convergence?

- General result (Moan, 2002)

$$\|\Omega_m\| \leq 2^{m-1} f_m \left(\int_{\tau_0}^{\tau} \|\mathcal{S}_2(\tau_1)\| d\tau_1 \right)^m$$

with $f_1 = 1$, $f_2 = \frac{1}{4}$, $f_3 = \frac{5}{72}$, $f_4 = \frac{11}{576}$, etc.

- $f_{m+1}/f_m \approx 0.1$ (not very rapid)

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Specific example

Spin 1/2 system in a rotating magnetic field that makes an angle α (constant) with the z axis with period of rotation $T = 2\pi/\omega$.

- Here $\varepsilon = 1/T$
- Hamiltonian

$$H(\tau) = \frac{1}{2}\gamma \vec{B}(\tau) \cdot \vec{\sigma}$$

- γ : gyromagnetic ratio
- Magnetic field $\vec{B}(\tau) = B(\sin \alpha \cos 2\pi\tau, \sin \alpha \sin 2\pi\tau, \cos \alpha)$
- σ_i : Pauli matrices
- The exact solution is known

Spin 1/2 system

$$\mathbf{S}_2(\tau) = i\pi \sin \alpha \begin{pmatrix} 0 & e^{-2i\beta\tau} \\ e^{2i\beta\tau} & 0 \end{pmatrix}$$

with $\beta = -\frac{\gamma B}{2\varepsilon} + \pi \cos \alpha$, and

$$\int_{\tau_0}^{\tau} \|\mathbf{S}_2(\tau_1)\|_2 d\tau_1 = \pi |\sin \alpha| (\tau - \tau_0)$$

which is always $< \pi$, since $0 \leq \tau - \tau_0 \leq 1$.

Magnus expansion in the adiabatic picture is always convergent

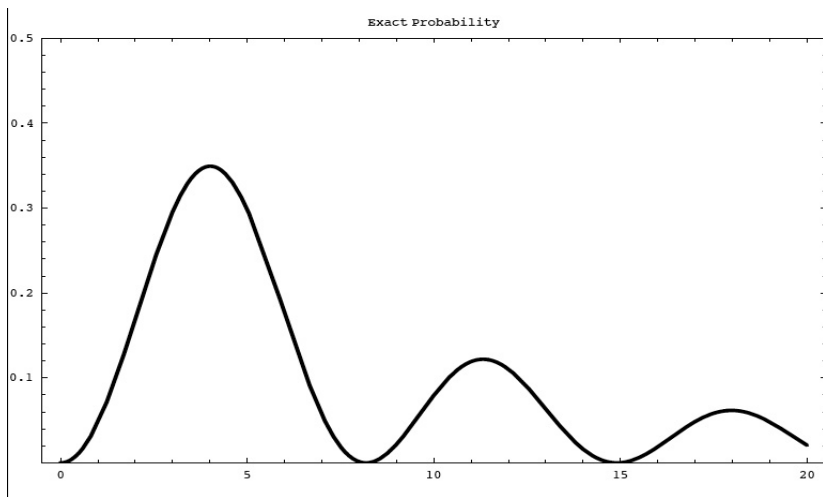
Transition probability

- Transition between the two eigenstates of H that belong to spin projections $\pm 1/2$ along the rotating magnetic field $\vec{B}(\tau)$.
- The exact result P_{ex} is known.
- P_{ex} vanishes in the adiabatic limit (no transition at all)
- We compare with the result achieved with the Magnus expansion
- It is very easy to compute any term $\Omega_k(\tau)$
- $P_{\text{M}}(\tau) = |(U_2(\tau))_{21}|^2$
- Numerical experiments: $\alpha = 2\pi/3$, $\tau_0 = 0$, $\tau = 1$.

Transition probability

- We compute up to $\Omega_{11}(\tau)$ and the corresponding $P_M(\tau)$ obtained with $\Omega^{[p]} = \sum_{i=1}^p \Omega_i$ up to $p = 11$
- No contribution from Ω_{2j}
- Compare with the exact result
- Gauge the quality of the different approximations as a function of $\xi \equiv \gamma B/\varepsilon$

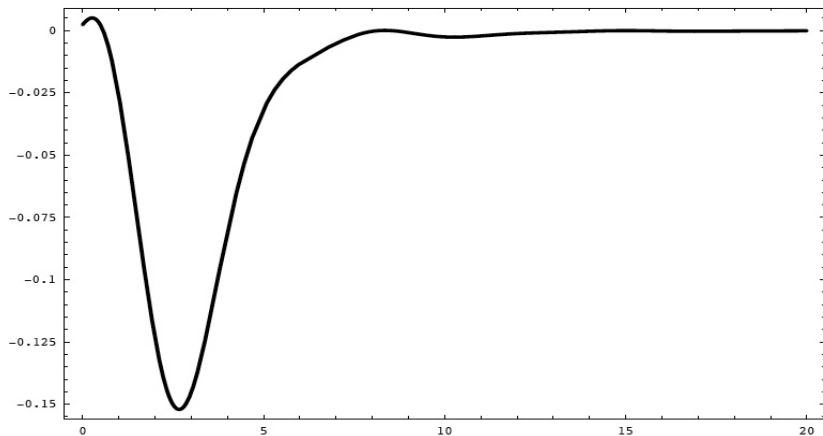
Exact transition probability vs. $\xi = \gamma B/\varepsilon$



Comparison Magnus – Exact result

| p | Diff. ($\xi = 10$) | Diff. ($\xi = 20$) |
|-----|------------------------|------------------------|
| 1 | -6.57×10^{-2} | 1.77×10^{-2} |
| 3 | 1.63×10^{-2} | 1.43×10^{-3} |
| 5 | -2.52×10^{-3} | 7.57×10^{-5} |
| 7 | 5.87×10^{-4} | 1.19×10^{-5} |
| 9 | -1.19×10^{-4} | -9.76×10^{-7} |
| 11 | 2.93×10^{-5} | 1.31×10^{-7} |

Error with $p = 5$ vs. $\xi = \gamma B/\varepsilon$



Remarks

- Velocity of convergence in Magnus consistent with theoretical estimates
- Very small errors for $\xi \geq 10$, even only with the first terms in the expansion
- Smaller errors with large ξ and more terms in Magnus
- Good description in the near-adiabatic regime

Conclusions

- Convergence of Magnus expansion assured in the adiabatic picture
- For the examples analyzed, the first terms in Magnus provide a good description in the near-adiabatic regime
- The approximation is expressed in terms of integrals
- In general, it will be difficult to compute exactly the integrals appearing in Ω_k , $k \geq 2$. So, what to do then?
- Integrand: highly oscillatory functions. Therefore, [Filon quadratures](#) are particularly suitable.
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- This approach should be competitive with other schemes (Jahnke et al.)
- Good results for (not so) small ε , and not only in the limit $\varepsilon \rightarrow 0$
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Conclusions

- Idea: either consider **only one** quadrature in the whole integration interval or divide the interval in a **small number** of subintervals and then apply Filon-like quadratures
- This approach should be competitive with other schemes (Jahnke et al.)
- Good results for (not so) small ε , and not only in the limit $\varepsilon \rightarrow 0$
- Work in progress...