Convergence of Time Splitting Methods for Quantum Dynamics in the Semiclassical Regime

François Golse

CMLS, École polytechnique, Paris

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Work in collaboration with Shi Jin and Thierry Paul
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Simple (Lie-Trotter) Time Splitting for Quantum Dynamics

Schrödinger eqn with unknown $\psi \equiv \psi(t,x) \in L^2(\mathbf{R}^d;\mathbf{C}) =: \mathfrak{H}$

$$i\hbar\partial_t\psi(t,x) = \underbrace{\left(-\tfrac{1}{2}\hbar^2\Delta_x + V(x)\right)}_{\mathcal{H}_\hbar}\psi(t,x)\,, \quad \psi(0,x) = \psi^{in}(x)$$

Simple time-splitting setting $\psi^0 := \psi^{in}$, define ψ^n for $n \geq 0$ by

$$\psi^{n+\frac{1}{2}} = \exp(\tfrac{1}{2}i\Delta t\hbar\Delta_x)\psi^n\,, \quad \psi^{n+1} = \exp\left(\tfrac{\Delta t}{i\hbar}V(x)\right)\psi^{n+\frac{1}{2}}$$

Error bound For $\psi^{in} \in H^1(\mathbf{R}^d)$ [Descombes-Thalhammer 2010]

$$\|\psi(n\Delta t,\cdot) - \psi^n\|_{\mathfrak{H}} \leq C(M, \|V\|_{W^{2,\infty}})\frac{\Delta t}{\hbar}$$

[Bao-Jin-Markowich 2003] **uniform** in $\hbar$ convergence of observables, without uniform in $\hbar$ error bound

Density Operators

State of a quantum system described by an operator on $\mathfrak{H} := L^2(\mathbf{R}^d)$

Example 1: pure state

$$R : \mathfrak{H} \ni \phi \mapsto \langle\psi|\phi\rangle\psi \quad \text{with } \|\psi\|_{\mathfrak{H}} = 1\,, \quad \text{denoted } |\psi\rangle\langle\psi|$$

Example 2: mixed state For ψ_n complete+orthonormal in $\mathfrak{H}$

$$R = \sum_{n\ge1} \lambda_n |\psi_n\rangle\langle\psi_n| \qquad \text{with } \lambda_n \ge 0\,, \quad \underbrace{\sum_{n\ge1} \lambda_n}_{=\mathrm{tr}_{\mathfrak{H}}(R)} = 1$$

Example 3: Töplitz density operator For $\mu \in \mathcal{P}(\mathbf{R}^d_q \times \mathbf{R}^d_p)$

$$\mathrm{OP}^T_\hbar[\mu] = \int |q,p\rangle\langle q,p|\mu(dqdp)\,, \qquad \underbrace{|q,p\rangle(x) = \frac{e^{-\frac{|x-q|^2}{2\hbar}+i\frac{p.x}{\hbar}}}{(\pi\hbar)^{d/4}}}_{\text{coherent state}}$$

Quantum Dynamics: Exact/Time-Split

Exact dynamics starting from R^{in}

$$R(t) = \exp(\tfrac{t\mathcal{H}}{i\hbar})R^{in}\exp(-\tfrac{t\mathcal{H}}{i\hbar})\,, \qquad \text{with } \mathcal{H} := -\tfrac{1}{2}\hbar^2\Delta_x + V(x)$$

Time-split dynamics starting from $R^0 = R^{in}$

$$R^{n+1} = \exp(\tfrac{\Delta t}{i\hbar}V)\exp(\tfrac{i\hbar\Delta t}{2}\Delta_x)R^n\exp(-\tfrac{i\hbar\Delta t}{2}\Delta_x)\exp(-\tfrac{\Delta t}{i\hbar}V)$$

Husimi function of a density operator R

$$\tilde{W}_\hbar[R] := \tfrac{1}{(2\pi\hbar)^d}\langle q,p|R|q,p\rangle = \text{ probability density on } \mathbf{R}^d_q \times \mathbf{R}^d_p$$

Problem to compare $\tilde{W}_\hbar[R(n\Delta t)]$ and $\tilde{W}_\hbar[R^n]$ **uniformly** in $\hbar$

Uniform in $\hbar$ Error Bound

Truncated Monge-Kantorovich distance for $\mu, \nu \in \mathcal{P}(\mathbf{R}^d_q \times \mathbf{R}^d_p)$

$$\text{dist}_1(\mu,\nu) := \max_{\substack{|\phi(q,p)-\phi(q',p')| \\ \leq \max(1,|(q,p)-(q',p')|)}} \left| \int \phi(\mu-\nu)(dqdp) \right|$$

Thm Let f^{in} be a probability density on $\mathbf{R}^{2d}$ with finite 2nd order moment, and set $R^{in} = \text{OP}^T_\hbar[f^{in}]$. Assume that $V \in W^{2,\infty}(\mathbf{R}^d)$ and set $\Lambda := \max(1, \text{Lip}(\nabla V))$. For each $T > 0$ and $\hbar > 0$

$$\text{dist}_1(\widetilde{W}_\hbar(R^n), \widetilde{W}_\hbar(R(n\Delta t)) \leq C\left[T, \Lambda, f^{in}\right] \Delta t^{1/3}, \quad 0 \leq n \leq [\tfrac{T}{\Delta t}]$$

Proof based on optimizing in $\hbar$ between the Descombes-Thalhammer error bound + another bound obtained by AP scheme methodology

AP Scheme Methodology

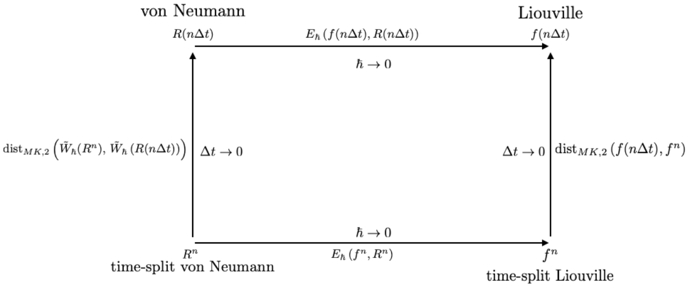

Figure: The horizontal arrows represent the semiclassical limit $\hbar \ll 1$ and the vertical arrows the convergence of the numerical scheme $\Delta t \ll 1$.

Comparing Quantum vs Classical Densities

A **coupling** of $f \equiv f(q,p)$ probability density with finite 2nd moment on $\mathbf{R}^d_q \times \mathbf{R}^d_q$ and R density operator on $\mathfrak{H}$ is

$$(q,p) \mapsto \Pi(q,p) = \Pi(q,p)^* \geq 0 \text{ s.t. } \begin{cases} \iint \Pi(q,p)dqdp = R \\ \operatorname{tr}_{\mathfrak{H}} \Pi(q,p) = f(q,p) \end{cases}$$

Pseudodistance between f and R

$$E_\hbar(f,R) = \inf_{\Pi} \left(\iint \operatorname{tr}_{\mathfrak{H}}(\Pi(q,p)^{1/2} C(q,p) \Pi(q,p)^{1/2}) dqdp \right)^{1/2}$$

with **quantum transport cost**

$$C(q,p) := \sum_{j=1}^{d} \left((q_j - x_j)^2 + (p_j + i\hbar\partial_{x_j})^2 \right)$$

Key Inequalities

General lower bound

$$E_\hbar(f,R)^2 \geq \max(d\hbar, \mathrm{dist}_{MK,2}(f,\tilde{W}_\hbar[R])^2 - d\hbar)$$

Upper bound for Töplitz densities

$$E_\hbar(f,\mathrm{OP}^T_\hbar[g])^2 \leq \mathrm{dist}_{MK,2}(f,g)^2 + d\hbar$$

Propagation if Φ_t :=Hamiltonian flow of $\frac{1}{2}|p|^2 + V(q)$, then

$$E_\hbar(f^{in}\circ\Phi_t, \exp(\tfrac{t\mathcal{H}}{i\hbar})R^{in}\exp(-\tfrac{t\mathcal{H}}{i\hbar})) \leq E_\hbar(f^{in},R^{in})e^{\frac{1}{2}t(1+\Lambda^2)}$$

Extensions

(1) Extension to **higher order** time-splitting methods — for instance, uniform $O(\Delta t^{2/3})$ error bound for Strang splitting if $V \in W^{3,\infty}(\mathbf{R}^d)$

(2) Extensions to other quantum dynamics possible (magnetic fields, Ehrenfest dynamics...)

(3) Fully discrete schemes not analyzed here, because at the moment, spatial discretization of wave functions in the semiclassical regime seems to require $O(\hbar^{1/2})$ "mesh" size (for Gaussian beam methods)

(4) Some major difficulties which remain to be solved
(a) singular potentials?
(b) boundary value problems?