On the convergence of a novel time slicing approximation for Feynman path integrals

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Memories from OPSO 2021 - Feynman path integrals

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Assumption (Feynman, 1948)

The integral kernel $u_t(x,y)$ of any Schrödinger propagator $U(t) = e^{-\frac{i}{\hbar}tH}$ with quantum Hamiltonian H can be represented as a ***path integral****:*

$$u_t(x,y) = \int e^{\frac{i}{\hbar}S[\gamma]}\mathcal{D}\gamma,$$

where $S[\gamma] = \int_0^t L(\gamma(\tau),\dot{\gamma}(\tau),\tau)d\tau$ is the ***action functional*** *(L being the classical Lagrangian) corresponding to a path γ satisfying $\gamma(0) = y$ and $\gamma(t) = x$.*

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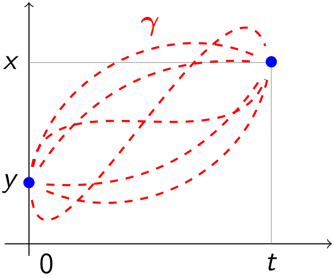

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- The **Trotter product formula**: under suitable assumptions on the potential V we have

$$U(t)f = e^{-\frac{i}{\hbar}t(H_0+V)}f = \lim_{n\to\infty} E_n(t)f, \quad f \in L^2(\mathbb{R}^d),$$

  where the **Feynman-Trotter approximate propagators** are

$$E_n(t) = \left(e^{-\frac{i}{\hbar}\frac{t}{n}H_0}e^{-\frac{i}{\hbar}\frac{t}{n}V}\right)^n.$$

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Combining the two results gives a representation of $U(t) = e^{-\frac{i}{\hbar}t(H_0+V)}$ as (strong) limit of a sequence of integral operators.

Memories from OPSO 2021 - convegence of kernels?

... the limit exists and we may write

$$K(b,a) = \lim_{\epsilon \to 0} \frac{1}{A} \int \cdots \int \int e^{\frac{i}{\hbar} S[b,a]} \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A} \qquad (\star)$$

[where $A = (2\pi i \hbar \epsilon / m)^{1/2}$ and $N\epsilon = t_b - t_a$] ...

... we shall write the sum over all paths in a less restrictive notation as

$$K(b,a) = \int_{t_a}^{t_b} e^{\frac{i}{\hbar} S[b,a]} \mathcal{D}x(t) \qquad (\star)$$

which we shall call a path integral.

— *Feynman and Hibbs, Quantum Mechanics and Path Integrals (1965)*

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... The Trotter product formula shows that the transition from ($\star$) to ($\star$) can be made rigorously on the level of operators rather than integral kernels, under suitable conditions on the potential V...

— *Folland, Quantum Field Theory - A Tourist Guide for Mathematicians (2008)*

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Set $\hbar = 1/2\pi$ for convenience. Our problem:

$$\begin{cases} i\partial_t \psi = 2\pi H_0 \psi \\ \psi(0,x) = f(x), \end{cases}$$

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where H_0 is the Weyl quantization of a real quadratic form $Q(x,\xi)$ on $\mathbb{R}^{2d}$ and V is the Fourier transform of a finite measure on $\mathbb{R}^d$.

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Nicola, Trapasso - Comm. Math. Phys. 2020

Let $e_{n,t}(x,y)$ and $u_t(x,y)$ be the integral kernels of $E_n(t)$ and $U(t)$ resp.

For any fixed $t \in \mathbb{R} \setminus \mathfrak{E}$ (= up to exceptional times) we have

$$e_{n,t},\ u_t \in C_b(\mathbb{R}^{2d}) \quad \text{and}$$

$$e_{n,t} \to u_t \ \text{ uniformly on compact subsets of } \mathbb{R}^{2d}.$$

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- $H_0 = Q^{\mathrm{w}}$ coincides with a **metaplectic operator** $\mu(S_t) \in \mathcal{U}(L^2(\mathbb{R}^d))$ associated with the classical flow $S_t \in \mathrm{Sp}(d, \mathbb{R})$ in phase space.

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- Except for a set $\mathfrak{E}$, $\mu(S_t)$ can be represented as an integral operator (a "quadratic" Fourier transform):

$$U_0(t)f(x) = c(t) \int_{\mathbb{R}^d} e^{2\pi i \Phi_t(x,y)} f(y) dy,$$

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- The quantum propagator evolves Gabor wave packets along the classical flow: for any $t \in \mathbb{R}$, $N \in \mathbb{N}$ there exists $C_{t,N} > 0$ s. t.

$$|\langle \mu(S_t)\pi(z)g, \pi(w)g \rangle| \leq C(1 + |w - S_t z|)^{-N}, \quad w, z \in \mathbb{R}^{2d},$$

where $g \in \mathcal{S}(\mathbb{R}^d)$ and $\pi(x, \xi)g(y) = e^{2\pi i y \cdot \xi} g(y - x)$, $(x, \xi) \in \mathbb{R}^{2d}$.

- The potential V (viewed as a function in $C_b(\mathbb{R}^d)$) has a peculiar phase space regularity. Precisely, its Gabor wave packet transform

$$\mathcal{V}_g V(x,\xi) = \langle V, \pi(x,\xi)g \rangle = \int_{\mathbb{R}^d} e^{-2\pi i y\cdot\xi} V(y)\overline{g(y-x)}dy$$

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- The Sjöstrand class is a Banach algebra of symbols: for every $\sigma \in M^{\infty,1}(\mathbb{R}^{2d})$, the Weyl pseudodifferential operator

$$\sigma^{\mathrm{w}} f(x) := \int_{\mathbb{R}^{2d}} e^{2\pi i (x-y)\cdot\xi} \sigma\left(\frac{x+y}{2}, \xi\right) f(y)\, dy d\xi$$

is bounded on $L^2(\mathbb{R}^d)$. Moreover, if $\sigma_1, \sigma_2 \in M^{\infty,1}(\mathbb{R}^{2d})$ then

$$\sigma_1^{\mathrm{w}} \sigma_2^{\mathrm{w}} = (\sigma_1 \# \sigma_2)^{\mathrm{w}}, \quad \sigma_1 \# \sigma_2 \in M^{\infty,1}(\mathbb{R}^{2d}).$$

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- The potential $V\times$ (viewed as a multiplication operator) is the Weyl quantization of $\sigma_V = V \otimes 1 \in M^{\infty,1}(\mathbb{R}^{2d})$.

- The Sjöstrand class is also a Banach algebra of complex-valued functions under pointwise multiplication.

Set $\rho_{t/n} := e^{-2\pi i \frac{t}{n}\sigma_V}$. Then $\rho_{t/n} \in M^{\infty,1}(\mathbb{R}^{2d})$ and there exists $\rho_0 \in M^{\infty,1}(\mathbb{R}^{2d})$ with $\|\rho_0\|_{M^{\infty,1}} \leq C(t)$ such that

$$e^{-2\pi i \frac{t}{n} V} = \rho_{t/n}^{\mathrm{w}} = I + 2\pi i \frac{t}{n} \rho_0^{\mathrm{w}}.$$

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- Metapletic operators combine well with (and only with!) Weyl operators - the symplectic covariance property:

$$\sigma^{\mathrm{w}} \mu(S) = \mu(S)(\sigma \circ S)^{\mathrm{w}}.$$

As a result, the Trotter approximation ops. can be expanded to obtain

$$E_n(t) = \left(e^{-2\pi i \frac{t}{n} H_0} e^{-2\pi i \frac{t}{n} V}\right)^n$$

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&= U_0(t)\rho^{\mathrm{w}}_{n,t},
\end{aligned}$$

for suitable $\rho_{n,t}$ in bounded subsets of $M^{\infty,1}$ (uniformly w.r.t. n), precisely

$$\sigma_{n,t} = \prod_{k=0}^{n-1}\left(1 + 2\pi i \frac{t}{n}\left(\rho_0 \circ S_{k\frac{t}{n}}\right)\right).$$

Operators of the form $T = \mu(S)\sigma^{\mathrm{w}}$ with $\sigma \in M^{\infty,1}(\mathbb{R}^{2d})$ are called generalized metaplectic operators associated with S - we write $T \in FIO(S)$. In particular, we have that $E_n(t) \in FIO(S_t)$.

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$$E_n(t)f(x) = c(t) \int_{\mathbb{R}^d} e^{2\pi i \Phi_t(x,y)} a_{n,t}(x,y) f(y) dy,$$

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  now with an extra amplitude $a_{n,t}(x,y) \in M^{\infty,1}(\mathbb{R}^{2d})$.

- $E_n(t)$ are still well localized in phase space near the graph of S_t:

$$|\langle E_n(t)\pi(z)g, \pi(w)g\rangle| \le H_{n,t}(w - S_t z),$$

  for some control function $H_{n,t} \in L^1(\mathbb{R}^{2d})$.

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Let $H = H_0 + V$ with $H_0 = Q^{\mathrm{w}} = \mu(S_t)$ as above and $V = \sigma_V^{\mathrm{w}}$ for some $\sigma_V \in M^{\infty,1}(\mathbb{R}^{2d})$ (e.g., $\sigma_V = V \otimes 1$ with $V \in M^{\infty,1}(\mathbb{R}^d)$ as before).

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This can be viewed using the standard perturbation method:

- Recast the problem in integral form (Duhamel):

$$\psi(t,x) = U_0(t)f(x) - 2\pi i \int_0^t U_0(t-\tau)\sigma_V^{\mathrm{w}}\psi(\tau,x)d\tau.$$

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- Switch to *interaction representation* with $\varphi(t,x) = U_0(-t)\psi(t,x)$, then use symplectic covariance and invariance of $M^{\infty,1}$:

$$\begin{aligned}\varphi(t,x) &= f(x) - 2\pi i \int_0^t U_0(-\tau)\sigma_V^{\mathrm{w}}U_0(\tau)\varphi(\tau,x)d\tau \\ &= f(x) - 2\pi i \int_0^t \underbrace{(\sigma_V \circ S_\tau)^{\mathrm{w}}}_{\in M^{\infty,1}}\varphi(\tau,x)d\tau,\end{aligned}$$

The solution of the previous Volterra integral equation is then

$$\varphi(t,x) = \alpha_t^{\mathrm{w}} f(x),$$

where the symbol α_t has a Dyson-Phillips expansion:

$$\begin{aligned}\alpha_t &= \mathcal{T} \exp\left(-2\pi i \int_0^t (\sigma_V \circ S_\tau) d\tau\right) \\ &:= 1 + \sum_{n\geq 1} (-2\pi i)^n \int_0^t \int_0^{\tau_1} \cdots \int_0^{\tau_{n-1}} \prod_{k=1}^{n} (\sigma_V \circ S_{\tau_k})\, d\tau_n \cdots d\tau_1.\end{aligned}$$

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To conclude,

$$\psi(t,x) = U_0(t)\varphi(t,x) = U_0(t)\alpha_t^{\mathrm{w}} f(x),$$

hence the claim:

$$U(t) = U_0(t)\alpha_t^{\mathrm{w}} \in FIO(S_t).$$

Another look at the Schrödinger propagator

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The resulting time-slicing approximation are then given by

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This proves that $\widetilde{E_n}(t) \in FIO(S_t)$, as expected.

Why this should be better?

Short summary: we are looking for *FIO*-type approximations of

$$U(t) = e^{-2\pi i t(H_0+V)} = U_0(t)\alpha_t^{\mathrm{w}} \in FIO(S_t),$$

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Two options so far, respectively Trotter-type or "Dyson-type" parametrices:

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They have a crucially different short-time approximation power!

$$\|\alpha_{t/n} - \rho_{t/n}\|_{M^{\infty,1}} \lesssim_t t/n, \qquad \|\alpha_{t/n} - \tilde{\rho}_{t/n}\|_{M^{\infty,1}} \lesssim_t (t/n)^2.$$

Main results - convergence of symbols

The better short-time behaviour allows one to obtain a nice control when compositions are taken into account: recall that

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The proof relies on the generalization of an ingenious argument introduced by D. Fujiwara to handle sophisticate path integral approximations obtained by oscillatory integral operators (Duke Math. J., 1980).

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hence

$$\|U(t) - \widetilde{E_n}(t)\|_{L^2\to L^2} \le \frac{C'(t)}{n}.$$

Main results - convergence of kernels, with rates!

Recall that *FIO*-ops. have an integral representation:

$$U(t)f(x)=\int_{\mathbb{R}^d} u_t(x,y)f(y)dy, \quad \widetilde{E_n}(t)f(x)=\int_{\mathbb{R}^d} \widetilde{e_{n,t}}(x,y)f(y)dy,$$

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Let $\Psi \in C_c^\infty(\mathbb{R}^{2d})$ be a real-valued bump function. Then

$$\|[u_t - \widetilde{e_{n,t}}]\Psi\|_{\mathcal{F}L^1} \lesssim_{t,\Psi} \|\alpha_t - \tilde{\rho}_{n,t}\|_{M^{\infty,1}}.$$

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For any compact subset $K \subset \mathbb{R}^{2d}$ and a bump function Ψ_K on K, we obtain locally uniform convergence of kernels:

$$\sup_{z\in K} |u_t(z) - \widetilde{e_{n,t}}(z)| \lesssim_{\Psi_K} \frac{C''(t)}{n}.$$

More details?

The talk is based on the papers:

Fabio Nicola and S. Ivan Trapasso

On the pointwise convergence of the integral kernels in the Feynman-Trotter formula.

Comm. Math. Phys. **376** (2020), no. 3, 2277–2299.

S. Ivan Trapasso

On the convergence of a novel family of time slicing approximation operators for Feynman path integrals.

Preprint arXiv:2107.00886 (2021)

Hear ye, hear ye!

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Thank you for your kind attention!