Feynman's Operational Calculus and the Evolution Equation

Lance Nielsen, Lorenzo Riva

Creighton University
Department of Mathematics

1. Introduction and background

- The FOC is an operational calculus introduced by physicist Richard Feynman in his 1951 paper *An Operator Calculus Having Applications in Quantum Electrodynamics*. It was born out of a need to compute functions of non-commuting operators, which arise frequently in quantum mechanics.
- In the 1951 paper, Feynman introduced three heuristic rules to compute such functions and determine the order in which the operators would act: assign time indexes to the operators, compute the function by treating the operators as if they commuted, and "disentangle" the resulting expression to restore the order of the operators. The abstract approach used here was developed later by B. Jefferies, M. L. Lapidus, G. W. Johnson, and L. Nielsen, starting from the early 80's.

2. Functions of operators

- An operator is a linear map between two vector spaces. Operators can be composed (or multiplied) together to form other operators. Example: an $m \times n$ matrix A is an operator that takes a vector in \mathbb{R}^n and returns a vector in \mathbb{R}^m . If A is a $m \times p$ matrix and if B is a $p \times n$ matrix, then A corresponds to a linear map $T_A : \mathbb{R}^p \to \mathbb{R}^m$ and B corresponds to a linear map $T_B : \mathbb{R}^n \to \mathbb{R}^p$. Matrix multiplication AB corresponds to a linear map $T_{AB} : \mathbb{R}^n \to \mathbb{R}^m$. But BA may not be defined!
- In a product, the operators act in succession from right to left: (AB)(x) = A(B(x)). If we have (AB)(x) = (BA)(x) for all x, then A and B are said to commute. Composition is, in general, non-commutative (think of matrices).
- Now, consider the function $f(x,y)=xy^2$ of complex variables x and y. Let A and B are operators: what can we say about f(A,B)? If A and B commute, then there's no ambiguity in writing $f(A,B)=AB^2$. If however they do not commute, then their order in the expression matters and one has to chose how to write that product: AB^2 , BAB, B^2A , $\frac{1}{3}AB^2+\frac{1}{3}BAB+\frac{1}{3}B^2A$ or any expression that would give back AB^2 if A and B commuted.

3. Feynman's heuristic rules

- To solve this problem, Feynman came up with three rules:
- 1. Attach "time indices" to the operators. An operator with an "earlier" (smaller) time index would act before, or to the right, of an operator with a "later" (larger) time index.
- 2. Compute the function of these operators by treating them as though they commute.
- 3. "Disentangle" the expression by restoring the conventional order of the operators.
- Of the disentangling process, Feynman states "The process is not always easy to perform and, in fact, is the central problem of this operator calculus." One should note that Feynman did not attempt to supply rigorous proofs of his results and, in fact, it is not always clear how Feynman's rules are to be applied, even heuristically.

Note on attaching indexes

 \bullet If A and B are operators, then we define

$$A(t_1)B(t_2) = egin{cases} AB & \text{if } t_2 < t_1 \\ BA & \text{if } t_1 < t_2 \\ \text{undefined} & \text{if } t_1 = t_2 \end{cases}$$

The most common way to attach a time index to A is through an integral:

$$A = \frac{1}{t} \int_0^t A(s) ds,$$

where A(s) = A for all $s \in [0, t]$.

• The integral in this example is the usual integral over the real line (i.e. with respect to Lebesgue measure), but a variety of different measures (and hence integrals) can be used, as we will see.

4. Exponential of operators and disentangling the exponential function

Consider the following differential equation:

$$\frac{\partial u}{\partial t} = Au \qquad u(0) = u_0,$$

where A is a matrix. Given its similarity to the differential equation that defines the exponential function, we write its solution as

$$u = u_0 e^{tA} := u_0 \sum_{k=0}^{\infty} \frac{(tA)^k}{k!},$$

where the last expression comes from the Taylor series of e^x . Note that, since A is a bounded operator, the series will always converge, and it is thus well defined. But what would happen if A was unbounded?

 Take, for example the heat or the Schrödinger equation (in natural units)

$$\frac{\partial u}{\partial t} = \Delta u, \quad \frac{\partial \Psi}{\partial t} = -i \left(-\frac{1}{2} \Delta + V \right) \Psi,$$

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_n^2}$ is the Laplacian, V is a potential function, and $i^2 = -1$. The operator $A = \frac{i}{2}\Delta$ is unbounded and (the operator of multiplication by -iV) B = -iV may be unbounded, and so e^{tA} and e^{tB} cannot defined using a power series. The operational calculus will allow us to evaluate expressions like $e^{t\Delta}e^{tV}$ in a rigorous fashion.

• We begin by disentangling a function of one unbounded operator A and one bounded operator, multiplication by V(s). A will be the infinitesimal generator of a strongly continuous (C_0) semigroup of operators: that is, a family $\{T(t)\}_{t\geq 0}$ of linear operators for which T(t)T(s)=T(t+s) for all $t,s\geq 0$ and T(0)=I, and

$$Ax = \lim_{t \searrow 0} \frac{T(t)x - x}{t}.$$

Furthermore, we usually write $T(t) = e^{tA}$.

• In particular, for $\zeta \in \mathbb{C}_+$, we set $A = \frac{H_0}{\zeta} = -\frac{1}{2\zeta}\Delta$ and we associate Lebesgue measure ℓ on [0,T] to A. We know that the

operator A is the generator of a strongly continuous semigroup with action

$$\left(e^{-tA}\varphi\right)(\xi) = \left(\frac{\zeta}{2\pi t}\right)^{d/2} \int_{\mathbb{R}^d} \varphi(u) \exp\left(-\frac{\zeta \|\xi - u\|^2}{2t}\right) du$$

for $\varphi \in L^2(\mathbb{R}^d)$ and $\xi \in \mathbb{R}^d$. By the Wiener integration formula, the above is equal to a function-space (or path) integral over $C_0^t = \{y: [0,t] \to \mathbb{R}^d | y(0) = 0 \text{ and } y \text{ is continuous} \}$ with respect to Wiener measure \mathfrak{m} :

$$\left(e^{-tA}\varphi\right)(\xi) = \int_{C_0^t} \varphi\left(\zeta^{-1/2}y(t) + \xi\right) \mathfrak{m}(dy).$$

- We also set $V(s) \in \mathcal{L}(L^2(\mathbb{R}^d))$ to be the operator of multiplication by a bounded function $V:[0,T]\times\mathbb{R}^d\to\mathbb{R}^d$: for $f\in L^2(\mathbb{R}^d)$ and $x\in\mathbb{R}^d,$ (V(s)f)(x)=V(s,x)f(x). We associate the measure $\lambda=\mu+\omega\delta_{\tau}$ to $V:\mu$ is a continuous measure on [0,t] and $\omega\delta_{\tau}$ is the Dirac point mass at $\tau\in[0,t]$ and weight ω .
- ullet Finally, we set $f(z_0,z_1)=e^{z_0}e^{z_1}$ and use the notation

$$f_{\ell;\lambda}^t(-H_0/\zeta;V) = \exp_{\ell,\lambda}^t \left(-t\frac{H_0}{\zeta} + \int_{[0,t]} V(s)\lambda(ds)\right);$$

the subscripts serve to emphasize the measure associated to each operator. Following Feynman's rules in a mathematically rigorous fashion, we obtain

$$\begin{split} &\left(\exp_{\ell,\lambda}^{t}\left(-t\frac{H_{0}}{\zeta}+\int_{[0,t]}V(s)\lambda(ds)\right)\varphi\right)(\xi) \\ &=\sum_{m=0}^{\infty}\frac{1}{m!}\sum_{k=0}^{m}\frac{m!\omega^{m-k}}{(m-k)!}\sum_{j=0}^{k}\int_{\Delta_{k;j}^{t}}\left(e^{-(t-s_{k})H_{0}/\zeta}V(s_{k})\cdots\right.\\ &\left.\cdots V(s_{j+1})e^{-(s_{j+1}-\tau)H_{0}/\zeta}[V(\tau)]^{m-k}e^{-(\tau-s_{j})H_{0}/\zeta}V(s_{j})\cdots\right.\\ &\left.\cdots V(s_{1})e^{-s_{1}H_{0}/\zeta}\varphi\right)(\xi)\mu^{k}(ds_{1},\ldots,ds_{k}) \\ &=\sum_{m=0}^{\infty}\frac{1}{m!}\sum_{k=0}^{m}\frac{m!\omega^{m-k}}{(m-k)!}\sum_{j=0}^{k}\int_{\Delta_{k;j}^{t}}\int_{C_{0}^{t}}V\left(\zeta^{-1/2}y(s_{1})+\xi,s_{1}\right)\cdots\right.\\ &\left.\cdots V\left(\zeta^{-1/2}y(s_{j+1})+\xi,s_{j+1}\right)\left[V\left(\zeta^{-1/2}y(\tau)+\xi,\tau\right)\right]^{m-k}\cdot\right.\\ &\left.V\left(\zeta^{-1/2}y(s_{j})+\xi,s_{j}\right)\cdots V\left(\zeta^{-1/2}y(s_{k})+\xi,s_{k}\right)\right.\\ &\left.\varphi\left(\zeta^{-1/2}y(t)+\xi\right)\mathfrak{m}(dy)\mu^{k}(ds_{1},\ldots,ds_{k})\right.\\ &=\int_{C_{0}^{t}}\sum_{m=0}^{\infty}\frac{1}{m!}\sum_{k=0}^{m}\frac{m!\omega^{m-k}}{(m-k)!k!}\left(\int_{[0,t]}V\left(\zeta^{-1/2}y(s)+\xi,s\right)\mu(ds)\right)^{k}\cdot\right.\\ &\left.\left[V\left(\zeta^{-1/2}y(\tau)+\xi,\tau\right)\right]^{m-k}\varphi(\zeta^{-1/2}y(t)+\xi)\mathfrak{m}(dy)\right.\\ &=\int_{C_{0}^{t}}\sum_{m=0}^{\infty}\frac{1}{m!}\left(\int_{[0,t]}V\left(\zeta^{-1/2}y(s)+\xi,s\right)(\mu+\omega\delta_{\tau})(ds)\right)^{m}\cdot\right.\\ &\left.\varphi(\zeta^{-1/2}y(t)+\xi)\mathfrak{m}(dy)\right.\\ &=\int_{C_{0}^{t}}\exp\left(\int_{[0,t]}V\left(\zeta^{-1/2}y(s)+\xi,s\right)\lambda(ds)\right)\varphi(\zeta^{-1/2}y(t)+\xi)\mathfrak{m}(dy)\right.\\ &=:K(t) \end{split}$$

5. Evolution Equation

• We also get an associated integral equation for K(t), called the *evolution equation*, which describes the evolution of the operator K. If we let

$$K_{\mathsf{dis}}(t) = \int_{C_0^t} \exp\left(\int_{[0,t]} V\left(\zeta^{-1/2}y(s) + \xi, s\right) \omega \delta_{\tau}(ds)\right) \cdot \varphi(\zeta^{-1/2}y(t) + \xi) \mathfrak{m}(dy)$$

be the disentangling K(t) using only the discrete parts of the measure, then

$$K(t) = K_{\text{dis}}(t) + \int_0^t e^{-(t-s)H_0/\zeta} V(s)K(s)\mu(ds).$$

6. Disentangling the exponential of other operators

• Let $A, B: [0,T] \to \mathcal{O}(C(\mathbb{C}^d))$ be continuous functions, where $\mathcal{O}(C(\mathbb{C}^d))$ is the space of all operators on continuous function on \mathbb{C}^d , defined by:

$$(A(s)\varphi)(x) = a(s)\varphi(b(x,s))$$
$$(B(s)\varphi)(x) = V(x,s)\varphi(x)$$

for $s \in [0,T]$. The functions $[0,T] \xrightarrow{a} \mathbb{C}$ and $\mathbb{C}^d \times [0,T] \xrightarrow{b,V} \mathbb{C}^d$, are such that $A(s), B(s) : C(\mathbb{C}^d) \to C(\mathbb{C}^d)$ for all $s \in [0,T]$. We have the following:

Lemma. Let A(s) and B(s) be defined as above. Then A(s)B(t)=B(t)A(s) for all $s,t\in[0,T]$.

• Since operators of this kind commute, we are interested in what their evolution equation looks like. By following the same procedures used to disentangle the exponential of the free Hamiltonian, we obtain:

Theorem 1. Let A(s) be the action of a (C_0) contraction semi-group such that, for some functions a and b, $(A(s)\varphi)(x) = a(s)\varphi(b(x,s))$ for all $\varphi \in C(\mathbb{C}^d)$, all $s \in [0,T]$, and all $x \in \mathbb{C}^d$. Let its generator be $-\alpha$, i.e. $e^{-t\alpha} = A(t)$, associated with Lebesgue measure ℓ . Let B(s) be the operator defined by $(B(s)\varphi)(x) = V(x,s)\varphi(x)$ for all $\varphi \in C(\mathbb{C}^d)$, all $s \in [0,T]$, and all $x \in \mathbb{C}^d$. Associate to B the measure $\lambda = \mu + \delta_\tau$, where μ is continuous and $\tau \in (0,T)$. Then for all $\varphi \in C(\mathbb{C}^d)$, $\xi \in \mathbb{C}^d$, and $t > \tau$ we have

$$\left(\exp_{\ell,\lambda}^{t} \left(-t\alpha + \int_{[0,t]} B(s)\lambda(ds)\right)\varphi\right)(\xi)$$

$$= a(t)\varphi(b(\xi,t)) \exp\left(\int_{[0,t]} V(b(\xi,t),s)\lambda(ds)\right)$$

$$= (e^{-t\alpha}\varphi)(\xi) \exp\left(\int_{[0,t]} V(b(\xi,t),s)\lambda(ds)\right).$$

This theorem tells us that operators that commute with a simple multiplication by a function are not affected by the disentangling; in fact, the the theorem can be read as $\exp(A + B) = \exp(A)\exp(B)$, which is not true for general operators.