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THE POINTWISE HELLMANN-FEYNMAN THEOREM

DAVID CARFÌ *

ABSTRACT. In this paper we study *from a topological point of view* the Hellmann-Feynman theorem of Quantum Mechanics. The goal of the paper is twofold:

- On one hand we emphasize the role of the strong topology in the classic version of the theorem in Hilbert spaces, for what concerns the kind of convergence required on the space of continuous linear endomorphisms, which contains the space of (continuous) observables.
- On the other hand we state and prove a *new pointwise version* of the classic Hellmann-Feynman theorem. This new version is not yet present in the literature and follows the idea of A. Bohm concerning the topology which is desiderable to use in Quantum Mechanics. It is indeed out of question that this *non-trivial* new version of the Hellmann-Feynman theorem is the ideal one - for what concerns the continuous observables on Hilbert spaces, both from a theoretical point of view, since it is the strongest version obtainable in this context - we recall that the pointwise topology is the coarsest one compatible with the linear structure of the space of continuous observables -, and from a practical point of view, because the pointwise topology is the easiest to use among topologies: it brings back the problems to the Hilbert space topology.

Moreover, we desire to remark that this basic theorem of Quantum Mechanics, in his most desiderable form, is deeply interlaced with two cornerstones of Functional Analysis: the *Banach-Steinhaus theorem* and the *Baire theorem*.

1. Introduction

1.1. The physical context. Let a quantum physical system have a Hamiltonian operator depending upon a real parameter; that is, assume that to the physical system has a function $H : I \to \mathcal{L}(\mathcal{H})$, denoted also by $z \mapsto H_z$, mapping each element z of an interval I of the real line into a Hamiltonian operator $H(z)$ (belonging to the space $\mathcal{L}(\mathcal{H})$ of continuous linear endomorphisms of a Hilbert space $\mathcal{H}$ which represents the space of states of the physical system itself). In these conditions, the Hellmann-Feynman theorem states the relationship between the derivative of the total energy of the system on a certain path of eigenstates, with respect to the parameter, and the expectation value (on the same path of eigenstates) of the derivative of the Hamiltonian, with respect to the same parameter. The theorem was proved independently by Hans Hellmann (1937) (see [1]) and Richard Feynman (1939) (see [2]); a more recent version of the proof can be found in [3].

1.2. The classic version of the theorem. The theorem in its classic form can be stated (in a very slicked up version) in the following way.

Theorem 1.1. *Let the structure $(\vec{X}, \langle.|.\rangle)$ be a vector space $\vec{X}$ endowed with a compatible Diracian scalar product $\langle.|.\rangle$ (i.e., an anti-Hermitian form). Moreover, assume that*

- *$z \mapsto H_z$ is a function mapping each point z of an interval I of the real line into a Hamiltonian operator H_z,*
- *$z \mapsto \eta(z)$ is a function mapping each point of I into an eigenvector of the Hamiltonian H_z,*
- *E_z is the eigenvalue (energy) of the Hamiltonian H_z corresponding to the eigenvector $\eta(z)$, for any point z of I, that is, it fulfills the equality $H_z(\eta(z)) = E_z\eta(z)$.*

Then, the equality $E'(z) = \langle\eta(z)|H'(z)\eta(z)\rangle$, holds true for every z in I.

The classic formal proof employs a trivial lemma based on the normalization condition of unit vectors, which reads as follows.

Lemma 1.1. *Let the normalization condition $\langle\eta(z)|\eta(z)\rangle = 1$ hold for every z in an interval I of the real line. Then, defining the function $\langle\eta|\eta\rangle : I \to \mathbb{R}$ by $z \mapsto \langle\eta(z)|\eta(z)\rangle$, it follows $\langle\eta|\eta\rangle'(z) = 0$, for every value z of the parameter.*

Proof. This lemma is trivial since the derivative of a constant function is zero. ■

Formal proof of the Hellmann-Feynman theorem. The formal proof of the Hellmann Feynman theorem follows through repeated application of Leibnitz rules (for different operations of multiplication) to the quantum expectation value of the Hamiltonian. Indeed, define the function $\langle\eta|H\eta\rangle : I \to \mathbb{R}$ by $z \mapsto \langle\eta(z)|H(z)\eta(z)\rangle$, it follows

$$\begin{aligned}
E'(z) &= \langle\eta|H\eta\rangle'(z) = \\
&= \langle\eta'(z)|H(z)\eta(z)\rangle + \langle\eta(z)|(H\eta)'(z)\rangle = \\
&= \langle\eta'(z)|H(z)\eta(z)\rangle + \langle\eta(z)|H(z)\eta'(z) + H'(z)\eta(z)\rangle = \\
&= \langle\eta'(z)|H(z)\eta(z)\rangle + \langle\eta(z)|H(z)\eta'(z)\rangle + \langle\eta(z)|H'(z)\eta(z)\rangle = \\
&= E(z)\langle\eta'(z)|\eta(z)\rangle + E(z)\langle\eta(z)|\eta'(z)\rangle + \langle\eta(z)|H'(z)\eta(z)\rangle = \\
&= E(z)\langle\eta|\eta\rangle'(z) + \langle\eta(z)|H'(z)\eta(z)\rangle = \\
&= \langle\eta(z)|H'(z)\eta(z)\rangle,
\end{aligned}$$

and the proof should be complete. ■

1.3. A critical view of the classic version. However, from a mathematical point of view some problem arises:

- it is not clear in what sense the operator function H is differentiable in order to guarantee the validity of the above Leibnitz rules, *especially in the case of the multiplication of an operator with a vector*.

There are essentially two candidate-topologies on the vector space $\mathcal{L}(\mathcal{H})$: the weak topology (the pointwise one) and the strong topology (the topology induced by the canonical norm of the vector space $\mathcal{L}(\mathcal{H})$);

and consequently:

- *it is not clear what are the assumptions which assure the validity of the formal above proof;*
- *it is not clear what are the assumptions which are usually considered in the applications of the Hellmann-Feynman theorem.*

Concerning the first point, in this paper we reach two results:

- we emphasize that the Hellmann-Feynman theorem holds if we endow the space of continuous linear operators $\mathcal{L}(\mathcal{H})$ with the strong topology. In other terms, the theorem holds if we endow the vector space $\mathcal{L}(\mathcal{H})$ with its *canonical Banach structure*, given by the uniform norm $\|.\|_{\mathcal{L}(\mathcal{H})}$ defined by $\|A\|_{\mathcal{L}(\mathcal{H})} = \sup_{\overline{B}(0_{\mathcal{H}},1)} \|A\|_{\mathcal{H}}$, and inducing the strong topology on the space $\mathcal{L}(\mathcal{H})$ (in the above definition, $\overline{B}(0_{\mathcal{H}}, 1)$ denotes the closed unit ball of the Hilbert space $\mathcal{H}$).
- we prove that the Hellmann-Feynman theorem holds yet if we endow the space of continuous linear endomorphisms with the weak topology, that is the pointwise topology. Recall that the pointwise topology is the locally convex topology induced by the family $p = (p_\psi)_{\psi\in X}$ of seminorms $p_\psi : \mathcal{L}(\mathcal{H}) \to \mathbb{R}$ defined by $A \mapsto \|A(\psi)\|_{\mathcal{H}}$.

Concerning the second point, *it is not an unmistakable circumstance to understand what is the kind of convergence used in the practical applications of the theorem*, at least for two reasons

- the formal proofs present in the current literature do not specify with respect to what topologies the adopted infinitesimal calculus must be employed;
- if, on one hand, probably the tacitly implicit topology in the space of continuous linear operator should be the strong one (since this topology is a simple Banachizable topology), on the other hand, it is true that *often*, in the standard approaches to the space of observables in Quantum Mechanics, the topology assumed in the discussions is considered the weak one (see for instance the well known treatise of A. Bohm [4]).

1.4. Conclusions. Concluding, noting that every explicit indication in the current proofs to some kind of topology (or norm) in the space $\mathcal{L}(\mathcal{H})$ of continuous linear operators *is anyhow absent*, it is not clear when and how the presented formal proofs are correct and (consequently) when and in what sense the theorem in object is correct.

This paper gives two answers to these questions:

- we state and prove the Hellmann-Feynman theorem in the case of strong topology on $\mathcal{L}(\mathcal{H})$ in a complete and mathematically correct way. Probably (as suggested by some authors) this is the version known and assumed in the literature of Quantum Mechanics (but it is not so easy to affirm this idea with certainty), however we hardly find a proof in which there is trace of the canonical norm of the space of observables. We shall call our formulation of the Hellmann-Feynman theorem (that employs the strong topology) *weak Hellmann-Feynman theorem*;

- we state and prove the Hellmann-Feynman theorem in the case of pointwise topology on the space $\mathcal{L}(\mathcal{H})$ in a complete and mathematically correct way. This new version *is much strong and handy* in the applications, since the verification of pointwise differentiability is natural and simple (employing only the topology on the Hilbert space $\mathcal{H}$). It follows the (already mentioned) Bohm idea on topology in Quantum mechanics. Moreover, the new version *implies the weak Hellmann-Feynman theorem*, since the strong differentiability implies the pointwise one. This version and the relative proof are certainly absent in the literature: this new version can be considered original. The proof is not straightforward as in the case of the weak version and it should be noticed that the it employs:

  1) general theorems regarding *equicontinuity in the context of Baire spaces*;

  2) the *Banach-Steinhaus theorem in his complete version* in the same context of Baire spaces, as corollary of the *First Ascoli's theorem*.

2. Leibnitz rule for a scalar product

In this section the structure $\mathcal{H} = (\overrightarrow{X}, (\cdot|\cdot))$ will be a real or complex pre-Hilbert space.

Proposition 2.1 (Leibnitz rule for scalar products). *Let I be an interval of the real line $\mathbb{R}$, let $\alpha, \beta : I \to X$ be two $\mathcal{H}$-differentiable curves in the Hilbert space $\mathcal{H}$ and let $(\alpha \mid \beta)$ be the function from the real line into the real line (the curve in $\mathbb{R}$) defined, for every point z in I, by $(\alpha \mid \beta)(z) = (\alpha(z) \mid \beta(z))$. Then, the function $(\alpha \mid \beta)$ is differentiable and the following Leibnitz equality holds $(\alpha \mid \beta)' = (\alpha' \mid \beta) + (\alpha \mid \beta')$.*

Proof. For any point z_0 of the interval I and any point z in I different from z_0, the difference quotient Q of the function $(\alpha \mid \beta)$ at the point z centered at the point z_0 is given by

$$\begin{aligned} Q(z) &= \frac{(\alpha(z) \mid \beta(z)) - (\alpha(z_0) \mid \beta(z_0))}{z - z_0} = \\ &= \frac{(\alpha(z) \mid \beta(z)) - (\alpha(z) \mid \beta(z_0))}{z - z_0} + \frac{(\alpha(z) \mid \beta(z_0)) - (\alpha(z_0) \mid \beta(z_0))}{z - z_0} = \\ &= \left(\alpha(z) \mid \frac{\beta(z) - \beta(z_0)}{z - z_0}\right) + \left(\frac{\alpha(z) - \alpha(z_0)}{z - z_0} \mid \beta(z_0)\right), \end{aligned}$$

thus, by applying the operator ${}^{\mathcal{H}}\lim_{z_0}$, and taking into account (especially for the first addendum of the last sum) that the scalar product is a *continuous bilinear form on the Hilbert space* $\mathcal{H}$, we have $(\alpha \mid \beta)'(z_0) = (\alpha(z_0) \mid \beta'(z_0)) + (\alpha'(z_0) \mid \beta(z_0))$. ■

As a trivial consequence of the preceding rule we obtain the following lemma.

Lemma 2.1. *Let $\psi : I \to X$ be an $\mathcal{H}$-differentiable curve in the Hilbert space $\mathcal{H}$ with unitary values. Then, we have $(\psi' \mid \psi) = -(\psi \mid \psi')$.*

Proof. By assumption, for any point z of the interval I, the vector $\psi(z)$ is with unitary norm, that is $(\psi \mid \psi)(z) = 1$. Thus the real function $(\psi \mid \psi)$ is a constant function on the interval I and then its derivative is zero, $(\psi \mid \psi)' = 0$. By applying the Leibniz rule we obtain $(\psi' \mid \psi) + (\psi \mid \psi') = 0$. ■

3. Strongly differentiable curves of continuous endomorphisms

Definition 3.1 (derivatives of a curve of operators). *Let I be an interval of the real line $\mathbb{R}$, let $\mathcal{H} = (\vec{X}, (\cdot|\cdot))$ be a Hilbert space and let $A : I \to \mathcal{L}(\mathcal{H})$ be a curve of linear and continuous operators on the Hilbert space $\mathcal{H}$. The curve A is said to be **strongly differentiable** if the following $(\mathbb{R}, \tau)$-limit*

$$^{\tau}\lim_{z\to z_0} \frac{A(z) - A(z_0)}{z - z_0}$$

*there exists in the topological space $(\mathcal{L}(\mathcal{H}), \tau)$, for any point $z_0 \in I$, where τ is the topology of uniform convergence on bounded sets, that is the topology of the canonical Banach space $(\mathcal{L}(\mathcal{H}), \|.\|_{\mathcal{L}(\mathcal{H})})$. In this case, for every point z_0 of the interval I, the operator $A'(z_0) : X \to X$ defined by the above τ-limit in $\mathcal{L}(\mathcal{H})$ is called **the strong derivative of the curve** A **at the point** z_0.*

4. Leibniz rule for continuous bilinear mappings

To prove the Leibniz rule for the canonical bilinear application $\langle ., . \rangle_{\mathcal{L}(\mathcal{H}),X}$ from $\mathcal{L}(\mathcal{H}) \times X$ into X defined by $(A, \psi) \mapsto A(\psi)$, with respect to the canonical norm of the space $\mathcal{L}(\mathcal{H})$, we recall the following general result.

Proposition 4.1 (Leibniz rule for bilinear mappings among Banach spaces). *Let $(\vec{E}, \|.\|)$, $(\vec{F}, \|.\|)$, $(\vec{G}, \|.\|)$ be three Banach spaces, let $[\cdot, \cdot] : E \times F \to G$, denoted by $(x, y) \mapsto [x, y]$, be a continuous bilinear mapping of the Banach space $(\vec{E} \times \vec{F}, \|.\|_\infty)$ into the Banach space $(\vec{G}, \|.\|)$. Then the mapping $[\cdot, \cdot]$ is (Frèchet) differentiable at every point (x, y) of the product $E \times F$ and moreover its (Frèchet) derivative at the point (x, y) is the linear mapping $[\cdot, \cdot]'_{(x,y)} : E \times F \to G$ defined by $(s, t) \mapsto [s, y] + [x, t]$.*

Proof. We must prove that, for any pair (x, y) in the product $E \times F$, it holds

$$\lim_{(s,t)\to 0} \frac{\|[x + s, y + t] - [x, y] - [x, t] - [s, y]\|}{\|(s, t)\|_\infty} = 0.$$

At this purpose, for any two pairs (x, y) and (s, t) of the product $E \times F$, we have (by bilinearity)

$$[x + s, y + t] - [x, y] - [x, t] - [s, y] = [s, t].$$

Since the mapping $[\cdot,\cdot]$ is *bilinear and continuous*, there is a real number $c>0$ such that

$$\|[s,t]\| < c\ \|s\|\ \|t\| .$$

For any real number $\varepsilon>0$, the relation

$$\sup(\|s\|,\|t\|) = \|(s,t)\|_\infty \le \varepsilon/c$$

implies that

$$\begin{aligned}
\|[x+s,y+t]-[x,y]-[x,t]-[s,y]\| &= \|[s,t]\| \le \\
&\le c\ \|s\|\ \|t\| \le \\
&\le c\ \|(s,t)\|_\infty\ \|(s,t)\|_\infty \le \\
&\le c(\varepsilon/c)\,\|(s,t)\|_\infty = \\
&\le \varepsilon\,\|(s,t)\|_\infty ,
\end{aligned}$$

which proves our assertion (by definition of limit). ■

At this point, the bilinear application $\langle .,.\rangle_{\mathcal{L}(\mathcal{H}),X} : \mathcal{L}(\mathcal{H})\times X\to X$ is continuous with respect to the product of the topologies induced by the norms $\|.\|_{\mathcal{L}(\mathcal{H})}$ and $\|.\|_{\mathcal{H}}$, indeed

$$\|A\,(v)\|_{\mathcal{H}} \le \|A\|_{\mathcal{L}(\mathcal{H})}\ \|v\|_{\mathcal{H}} ,$$

so, applying the preceding result and the chain rule, we obtain immediately the following theorem, however we will give another direct proof.

Theorem 4.1 (Leibnitz rule for the image of a curve). *Let $\mathcal{H}=(\overrightarrow{X},(\cdot|\cdot))$ be a Hilbert space, let $\psi : I\to X$ be a differentiable curve in the Hilbert space $\mathcal{H}$ and let $A : I\to\mathcal{L}(\mathcal{H})$ be a strongly differentiable curve of continuous endomorphisms on $\mathcal{H}$ (i.e., a differentiable curve in the canonical Banach space $(\mathcal{L}(\mathcal{H}),\|.\|_{\mathcal{L}(\mathcal{H})})$). Let $A\,(\psi)$ be the curve in the Hilbert space $\mathcal{H}$ defined by $A\,(\psi)\,(z)=A(z)\psi(z)$, for every point z of the interval I. Then*

- *the curve $A\,(\psi)$ is differentiable in the space $\mathcal{H}$;*
- *the following Leibnitz rule holds true $A(\psi)'=A'(\psi)+A(\psi')$.*

Proof. Let Q be the difference quotient of the curve $A\,(\psi)$ centered at z_0. We have, for any point z of the interval I,

$$\begin{aligned}
Q(z) &= \frac{A\,(\psi)\,(z)-A\,(\psi)\,(z_0)}{z-z_0} = \\
&= \frac{A\,(z)\,(\psi\,(z))-A\,(z_0)\,(\psi\,(z_0))}{z-z_0} = \\
&= \frac{A\,(z)\,\psi\,(z)-A\,(z_0)\,\psi\,(z)}{z-z_0} + \frac{A\,(z_0)\,\psi\,(z)-A\,(z_0)\,\psi\,(z_0)}{z-z_0} = \\
&= \frac{A\,(z)-A\,(z_0)}{z-z_0}\psi\,(z) + A\,(z_0)\,\frac{\psi\,(z)-\psi\,(z_0)}{z-z_0},
\end{aligned}$$

the two terms of the last member have a limit at z_0 with respect to the topology of the Hilbert space $\mathcal{H}$; indeed, by the continuity of the bilinear application $\langle .,.\rangle_{\mathcal{L}(\mathcal{H}),X}$, the differentiability of the curve A and the continuity of the curve ψ the first limit is

$$^{\mathcal{H}}\lim_{z\to z_0}\frac{A(z)-A(z_0)}{z-z_0}\psi(z)=A'(z_0)\,\psi(z_0)\,;$$

the second limit, by the continuity of the operator $A(z_0)$ and by the differentiability of the curve ψ in z_0, is $A(z_0)\,(\psi'(z_0))$, so we obtain

$$^{\mathcal{H}}\lim_{z\to z_0}\frac{A(\psi)(z)-A(\psi)(z_0)}{z-z_0}=A'(z_0)\,\psi(z_0)+A(z_0)\,\psi'(z_0)\,,$$

in other words the curve $A(\psi):I\to X$ is differentiable on the interval I, with respect to the topology of the Hilbert space $\mathcal{H}$, and we have the following Leibnitz rule $A(\psi)'=A'(\psi)+A(\psi')$, as we desired. ■

5. Hermitian operators

We recall that if A is an endomorphism upon a pre-Hilbert space $\mathcal{H}$, the mean value $\langle A\rangle_\psi$ of the operator A on a state ψ of the pre-Hilbert space is defined by the scalar product $(A(\psi)\mid\psi)$.

Proposition 5.1. *Let A be a Hermitian endomorphism upon a pre-Hilbert space $\mathcal{H}$. Then, the mean value $\langle A\rangle_\psi$ of the operator A on a state ψ of the pre-Hilbert space is real.*

Proof. We have $(A(\psi)\mid\psi)=(\psi\mid A(\psi))=\overline{(A(\psi)\mid\psi)}$, and then the mean value $\langle A\rangle_\psi=(A(\psi)\mid\psi)$ is real. ■

Proposition 5.2. *Let A be an Hermitian endomorphism on a pre-Hilbert space $\mathcal{H}$. Then, the eigenvalues of A are real numbers.*

Proof. Since A is Hermitian, for every pair of vectors α and β of the pre-Hilbert space $\mathcal{H}$, we have $(A(\alpha)\mid\beta)=(\alpha\mid A(\beta))$. If α is an eigenvector of the operator A with eigenvalue $a\in\mathbb{C}$, we have

$$(A(\alpha)\mid\alpha)=(a\alpha\mid\alpha)=a\,(\alpha\mid\alpha)=a\,\|\alpha\|^2\,,$$

and, by hermiticity

$$\begin{aligned}(A(\alpha)\mid\alpha)&=(\alpha\mid A(\alpha))=\\&=\overline{(A(\alpha)\mid\alpha)}=\\&=\overline{(a\alpha\mid\alpha)}=\\&=\overline{a\,(\alpha\mid\alpha)}=\\&=\overline{a}\,\|\alpha\|^2\end{aligned}$$

so $\overline{a}\,\|\alpha\|^2=a\,\|\alpha\|^2$, and hence (since α is different from zero) $a=\overline{a}$, that is $a\in\mathbb{R}$. ■

Remark 5.1 (on the structures of the set of Hermitian endomorphisms). If A and B are two Hermitian operators on a pre-Hilbert space $\mathcal{H} = (\vec{X}, (.|.))$, for every pair of vectors v, w of the space and for each complex number c, we have

$$((cA)v|w) = (cA(v)|w) = c(Av|w) = c(v|Aw) = (v|(\bar{c}A)w),$$

and so, if c is a real number, the endomorphism cA is also Hermitian. Moreover, in the same above conditions, we have also

$$((A+B)v|w) = (Av|w) + (Bv|w) = (v|Aw) + (v|Bw) = (v|(A+B)w).$$

We can conclude that the set ${}^{H}End(\mathcal{H})$ of linear and Hermitian operators is a linear subspace of the *real* vector space $\overrightarrow{End}_{\mathbb{R}}(\mathcal{H})$ of endomorphisms on the complex pre-Hilbert space $\mathcal{H}$, not of the complex vector space $\overrightarrow{End}_{\mathbb{C}}(\mathcal{H})$, since it is an antilinear subspace of the space $\overrightarrow{End}_{\mathbb{C}}(\mathcal{H})$.

Remark 5.2 (on the convergent sequences of Hermitian endomorphisms). Let A be a sequence of Hermitian operators on a pre-Hilbert space $\mathcal{H}$ and assume that A is pointwise converging to a linear operator L. Then we have, for any two vectors v and w of the pre-Hilbert space $\mathcal{H}$, $(A_n v|w) = (v|A_n w)$ and, by continuity of the scalar product (with respect to the topology of the pre-Hilbert space $\mathcal{H}$),

$$\begin{aligned}(Lv|w) &= ({}^{\mathcal{H}}\lim_{n\to\infty}(A_n v)|w) = \\ &= \lim_{n\to\infty}(A_n v|w) = \\ &= \lim_{n\to\infty}(v|A_n w) = \\ &= (v|{}^{\mathcal{H}}\lim_{n\to\infty}(A_n w)) = \\ &= (v|Lw),\end{aligned}$$

consequently the limit of a pointwise convergent sequence of Hermitian endomorphisms is an Hermitian endomorphism.

Remark 5.3 (on the derivative of a curve of Hermitian endomorphisms). Is the derivative of a curve of Hermitian endomorphisms a curve of Hermitian endomorphisms too? Gathering all the preceding results, we can deduce that the pointwise derivative (and consequently the strong derivative) of a curve of (continuous) observables is an observable, since the pointwise derivative $A'(z)$ is the pointwise limit of a sequence of linear, continuous and Hermitian operators, namely the sequence

$$\left(\frac{A(z+1/n) - A(z)}{1/n}\right)_{n\in\mathbb{N}_>}.$$

As we will see better later, the derivative $A'(z)$ belongs to the space of linear and continuous operators $\mathcal{L}(\mathcal{H})$, for every real z, by the Banach-Steinhaus theorem, if $\mathcal{H}$ is a *Hilbert space*: the completeness is necessary to apply the *Baire theorem*.

6. The weak Hellmann-Feynman theorem

Now we can state and prove the Hellmann-Feynman theorem in the case of strong differentiability.

Theorem 6.1 (Hellmann-Feynman weak version). *Let the algebraic structure* $\mathcal{H} = (\vec{X}, (\cdot|\cdot))$ *be a complex Hilbert space, let* $A : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ *be a strongly differentiable curve of continuous linear operators, let* $\psi : \mathbb{R} \to X$ *be an* $\mathcal{H}$*-differentiable curve of unitary vectors in* $\mathcal{H}$ *and let* $a : \mathbb{R} \to \mathbb{C}$ *be a differentiable curve in the complex plane* $\mathbb{C}$*. Moreover, suppose that*

- *the operator* $A(z)$ *is Hermitian, for all* $z \in \mathbb{R}$*;*
- *the vector* $\psi(z)$ *is an eigenvector of the operator* $A(z)$*, for each real* z*, with respect to the eigenvalue* $a(z)$*; in other terms, let the equality* $A(z)\psi(z) = a(z)\psi(z)$*, hold for every* $z \in \mathbb{R}$*.*

Then, for every real z*, we have* $(\psi(z) \mid A'(z)\psi(z)) = a'(z)$*. In other terms, putting* $\langle A' \rangle_\psi (z) := \langle A'(z) \rangle_{\psi(z)}$*, for every real* z*, the functional equality* $\langle A' \rangle_\psi = a'$*, holds true.*

Proof. By assumption, we have $A(\psi) = a\psi$, where, as we already said, the image of the curve ψ by the curve of operators A is the curve $A(\psi) : \mathbb{R} \to X$ defined by $z \mapsto A(z)\psi(z)$. We have obviously $(\psi \mid A(\psi)) = (\psi \mid a\psi) = a(\psi \mid \psi) = a$. Now, by strong derivation,

$$\begin{aligned}
(\psi \mid A(\psi))' &= (\psi' \mid A(\psi)) + \left(\psi \mid A(\psi)'\right) = \\
&= (\psi' \mid A(\psi)) + (\psi \mid A'(\psi) + A(\psi')) = \\
&= (\psi' \mid A(\psi)) + (\psi \mid A'(\psi)) + (\psi \mid A(\psi')) = \\
&= (\psi' \mid a\psi) + (\psi \mid A'(\psi)) + (A(\psi) \mid \psi') = \\
&= \overline{a}(\psi' \mid \psi) + (\psi \mid A'(\psi)) + (a\psi \mid \psi') = \\
&= a(\psi' \mid \psi) + (\psi \mid A'(\psi)) + a(\psi \mid \psi') = \\
&= a[(\psi' \mid \psi) + (\psi \mid \psi')] + (\psi \mid A'(\psi)) = \\
&= a0 + (\psi \mid A'(\psi)),
\end{aligned}$$

and so $(\psi \mid A(\psi))' = (\psi \mid A'(\psi))$. Concluding, since $(\psi \mid A(\psi)) = a$, we have

$$(\psi \mid A'(\psi)) = (\psi \mid A(\psi))' = a',$$

as we desired. ■

7. Pointwise differentiable curves of continuous endomorphisms

Definition 7.1 (pointwise derivative of a curve of operators). *Let* I *be an interval of the real line* $\mathbb{R}$*, let* $\mathcal{H} = (\vec{X}, (\cdot|\cdot))$ *be a Hilbert space and let* $A : I \to \mathcal{L}(\mathcal{H})$ *be a* *curve of linear and continuous operators of the Hilbert space $\mathcal{H}$. The curve A is said to be* ***pointwise differentiable*** *if the following $(\mathbb{R},\mathcal{H})$-limit*

$$^{(\mathbb{R},\mathcal{H})}\mathrm{lim}_{z\to z_0}\frac{A(z)-A(z_0)}{z-z_0}(v)$$

exists (in the Hilbert space $\mathcal{H}$) for any point z of the interval I and any vector $v \in X$. In this case, for every point z_0 of the interval I, the operator $A'(z_0) : X \to X$ defined by

$$v \mapsto \ ^{(\mathbb{R},\mathcal{H})}\mathrm{lim}_{z\to z_0}\frac{A(z)-A(z_0)}{z-z_0}(v)$$

is called ***the pointwise (weak) derivative of the curve*** A ***at the point*** z.

At this stage we don't know neither if the pointwise derivative A' is a linear and continuous operator. Fortunately, the Banach-Steinhaus theorem gives us an answer to the problem, but before to prove the claim we devote the following section to the equicontinuity and the Banach-Steinhaus theorem.

8. Equicontinuity and the Banach-Steinhaus theorem

Let E_τ be a topological space and let (F, d) be a semimetric space with family of semimetrics $d = (d_j)_{j\in J}$. We recall two notions.

- An application f of E into F is *continuous at a point* x_0 of E, *with respect to the pair of structures* (τ, d), if and only if for any index j in J the function f is continuous at the point x_0 with respect to the pair (τ, d_j).

In other terms, f is continuous at a point x_0 of E, with respect to the pair of structures (τ, d), if and only if, for any index j in J and for every positive real $r > 0$, there exists a neighborhood U of the point x_0 in the topological space E_τ such that the image $f(U)$ is contained in the open ball $B_{d_j}(f(x_0), r)$.

- Analogously, a set $\mathcal{A}$ of applications of E into F is *equicontinuous at a point* x_0 of E, *with respect to the pair of structures* (τ, d), if and only if for any index j in J the set of functions $\mathcal{A}$ is equicontinuous at the point x_0 with respect to the pair (τ, d_j).

In other terms, $\mathcal{A}$ is equicontinuous at a point x_0 of E, with respect to the pair of structures (τ, d), if and only if, for any index j in J and for every positive real $r > 0$, there exists a neighborhood U of the point x_0 (in the topological space E_τ) such that, for any application f in $\mathcal{A}$, the image $f(U)$ is contained in the open ball $B_{d_j}(f(x_0), r)$.

Theorem 8.1 (Banach-Steinhaus). *Let $\overrightarrow{E}_\sigma$ and $\overrightarrow{F}_\tau$ be two topological vector spaces and let the topological space E_σ be a Baire space. Let u be a pointwise convergent sequence of continuous linear mappings from the first space $\overrightarrow{E}_\sigma$ into the second space $\overrightarrow{F}_\tau$. Then,*

- *the sequence u converges to a linear and continuous operator,*
- *the sequence u is equicontinuous.*

9. Continuity of the pointwise derivative

Theorem 9.1 (continuity of the pointwise derivative $A'(z)$). *Let I be an interval of the real line $\mathbb{R}$, let $\mathcal{H} = (\vec{X}, (\cdot|\cdot))$ be a Hilbert space and let $A : I \to \mathcal{L}(\mathcal{H})$ be a pointwise differentiable curve of linear and continuous operators of the Hilbert space $\mathcal{H}$. Then,*

- *the pointwise derivative $A'(z)$ belongs to the space of linear and continuous operators $\mathcal{L}(\mathcal{H})$, for every real z,*
- *moreover, the family of difference quotients centered at a point z_0 of the interval I is locally equicontinuous at z_0 in every bounded neighborhood of z_0.*

Proof. **Continuity.** Since a Hilbert space is a Baire space, and since the pointwise derivative $A'(z)$ is the pointwise limit of a sequence of linear and continuous operators, namely the sequence

$$\left(\frac{A(z+1/n) - A(z)}{1/n}\right)_{n\in\mathbb{N}},$$

$A'(z)$ belongs to the space of linear and continuous operators $\mathcal{L}(\mathcal{H})$, for every real z, by the Banach-Steinhaus theorem. **Local equicontinuity.** Again for the Banach-Steinhaus theorem, the above sequence is equicontinuous. For the same reason, if z_0 is a point of the interval I and V is a bounded neighborhood of the point z_0 the closure C of V is *compact*, the disconnected curve

$$Q : C\setminus\{z_0\} \to \mathcal{L}(\mathcal{H}) : z \mapsto \frac{A(z) - A(z_0)}{z - z_0},$$

viewed as a family of continuous linear operators is equicontinuous. Indeed, we have to prove that, for any vector v of the Hilbert space, the family of real numbers

$$(\|Q(z)(v)\|)_{z\in C\setminus\{z_0\}}$$

is bounded in the real line. For, by limit definition, there is a positive real r such that, for each z in the pierced open ball $B^{\neq}(z_0, r)$, the following inequality holds true

$$\|Q(z)(v) - A'(v)\| < 1,$$

from which we deduce the boundness of the function $B^{\neq}(z_0, r) \to \mathbb{R} : z \mapsto \|Q(z)(v)\|$, in fact

$$\|Q(z)(v)\| \le \|Q(z)(v) - A'(v)\| + \|A'(v)\| < 1 + \|A'(v)\|;$$

for the remaining part of the index set $C\setminus\{z_0\}$, that is the compact $K = C\setminus B^{\neq}(z_0, r)$, we have

$$\|Q(z)(v)\| \le M := \sup_{t\in K} \|Q(t)(v)\|,$$

by the Weierstrass theorem; consequently, we have

$$\sup_{t\in C\setminus\{z_0\}} \|Q(t)(v)\| \le M + 1 + \|A'(v)\|,$$

and the equicontinuity follows from the Banach Steinhaus theorem. ■

10. Two convergence lemmas via equicontinuity

Theorem 10.1. *Let E_τ be a topological space and let (F, d) be a semimetric space with family of semi-metrics $d = (d_i)_{j\in J}$. Let $f = (f_n)_{n\in\mathbb{N}}$ be a sequence of applications from E into F, and let $x = (x_n)_{n\in\mathbb{N}}$ be a sequence of points of E. Assume that*

- *the sequence x converges to a point x_* of E,*
- *the sequence f converges pointwise to a function f_* of ${}^E F$,*
- *the sequence f is equicontinuous.*

Then the sequence $f(x)$ in F defined, for any natural number n, by $f(x)_n = f_n(x_n)$, converges to the point $f_*(x_*)$ in the semimetric space (F, d).

Proof. We have to prove that, for any index j of J, the sequence $f(x)$ converges in the pseudometric space (F, d_j) to the point $f_*(x_*)$. For, we have

$$d_j(f_n(x_n), f_*(x_*)) \leq d_j(f_n(x_n), f_n(x_*)) + d_j(f_n(x_*), f_*(x_*)),$$

now, since the sequence f pointwise converges to the function f_*, the second term on the right side converges to 0. On the other hand, since the sequence f is equicontinuous, for each $r > 0$, there is a neighborhood U of x_* such that, for each natural n and for each point e in U, it holds the inequality $d_j(f_n(e), f_n(x_*)) < r$; taking into account that there is a natural n_0 such that, for any n greater than n_0, the point x_n belongs to the neighborhood U, we have that

$$\lim_{n\to\infty} d_j(f_n(x_n), f_n(x_*)) = 0,$$

and the theorem is proved. ■

Corollary 10.1. *Let E_τ be a topological space and let (F, d) be a semimetric space with family of semi-metrics $d = (d_j)_{j\in J}$. Let H be a subset of the real line $\mathbb{R}$, let $f = (f_h)_{h\in H}$ be a family of applications from E into F and let $x = (x_h)_{h\in H}$ be a family of points of E. Assume that*

- *h_0 is an accumulation point of the set H,*
- *the family x converges to a point x_* of E at the real h_0,*
- *the family f converges pointwise (in E) to a function f_* of ${}^E F$, at the real h_0,*
- *the sequence f is locally equicontinuous at h_0, in the sense that there is an open ball $V = B(h_0, r)$ such that the restriction of the family f to the intersection $V \cap H$ is an equicontinuous family.*

Then the family $f(x)$ in F defined, for any point h of H, by $f(x)_h = f_h(x_h)$, converges to the point $f_*(x_*)$ in the semimetric space (F, d).

Proof. It is enough to prove that, for every sequence $h = (h_n)_{n\in\mathbb{N}}$ of real numbers in H converging to h_0, it holds

$$^d\lim_{n\to\infty} f_{h_n}(x_{h_n}) = f_*(x_*),$$

and this follows immediately from the above theorem applied to the subfamily $(f_h)_{h\in V\cap H}$, taking into account that such sequences h must be eventually in the ball V. ■

11. Leibnitz rule for the pointwise derivative

Theorem 11.1 (Leibnitz rule for the image of a curve). *Let $\mathcal{H} = (\vec{X}, (. \mid .))$ be a Hilbert space, let $\psi : I \to X$ be a differentiable curve in the Hilbert space $\mathcal{H}$ and let $A : I \to \mathcal{L}(\mathcal{H})$ be a pointwise differentiable curve of continuous endomorphisms on $\mathcal{H}$. Let $A(\psi)$ be the curve in the Hilbert space $\mathcal{H}$ defined by $A(\psi)(z) = A(z)\psi(z)$, for every point z of the interval I. Then*

- *the curve $A(\psi)$ is differentiable in the space $\mathcal{H}$;*
- *the Leibnitz rule $A(\psi)' = A'(\psi) + A(\psi')$ holds true .*

Proof. Let Q be the difference quotient of the curve $A(\psi)$ centered at z_0. We have, for any point z of the interval I,

$$\begin{aligned} Q(z) &= \frac{A(\psi)(z) - A(\psi)(z_0)}{z - z_0} = \\ &= \frac{A(z)(\psi(z)) - A(z_0)(\psi(z_0))}{z - z_0} = \\ &= \frac{A(z)\psi(z) - A(z_0)\psi(z)}{z - z_0} + \frac{A(z_0)\psi(z) - A(z_0)\psi(z_0)}{z - z_0} = \\ &= \frac{A(z) - A(z_0)}{z - z_0}\psi(z) + A(z_0)\frac{\psi(z) - \psi(z_0)}{z - z_0}, \end{aligned}$$

the two terms of the last member have a limit at z_0 with respect to the topology of the Hilbert space $\mathcal{H}$; indeed, the family of difference quotients is locally equicontinuous at z_0 by the theorem 9.1, so we can apply the corollary 10.1, taking into account the pointwise differentiability of the curve A and the continuity of the curve ψ, the first limit is

$$^{\mathcal{H}}\lim_{z\to z_0} \frac{A(z) - A(z_0)}{z - z_0}\psi(z) = A'(z_0)\psi(z_0);$$

the second limit, by the continuity of the operator $A(z_0)$ and by the differentiability of the curve ψ in z_0, is $A(z_0)(\psi'(z_0))$. So we obtain

$$^{\mathcal{H}}\lim_{z\to z_0} \frac{A(\psi)(z) - A(\psi)(z_0)}{z - z_0} = A'(z_0)\psi(z_0) + A(z_0)\psi'(z_0),$$

in other words the curve $A(\psi)$ is differentiable on the interval I (with respect to the topology of $\mathcal{H}$) and we have the following Leibnitz rule $A(\psi)' = A'(\psi) + A(\psi')$, as we desired. ■

12. The strong Hellmann-Feynman theorem

Theorem 12.1 (Hellmann-Feynman strong version). *Let the algebraic structure $\mathcal{H} = (\vec{X}, (\cdot|\cdot))$ be a complex Hilbert space, let $A : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ be a pointwise differentiable curve of continuous linear operators, let $\psi : \mathbb{R} \to X$ be an $\mathcal{H}$-differentiable curve of unitary vectors in $\mathcal{H}$ and let $a : \mathbb{R} \to \mathbb{C}$ be a differentiable curve in the complex plane $\mathbb{C}$. Moreover, suppose that*

- *the operator $A(z)$ is Hermitian, for all $z \in \mathbb{R}$;*
- *the vector $\psi(z)$ is an eigenvector of the operator $A(z)$, for each real z, with respect to the eigenvalue $a(z)$; in other terms, let the equality $A(z)\psi(z) = a(z)\psi(z)$, hold for every $z \in \mathbb{R}$.*

Then, for every real z, we have $(\psi(z) \mid A'(z)\psi(z)) = a'(z)$. In other terms, putting $\langle A'\rangle_\psi(z) := \langle A'(z)\rangle_{\psi(z)}$, for every real z, the functional equality $\langle A'\rangle_\psi = a'$, holds true.

Proof. We have again at disposal the Leibnitz rules, so we can follow the formal classic proof. ■

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* Università degli Studi di Messina
Dipartimento di Economia, Statistica, Matematica e Sociologia "W. Pareto" (DESMAS)
Via dei Verdi, 75
98122 Messina, Italy

E-mail: davidcarfi71@yahoo.it

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