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Application of functional derivatives to analysis of complex systems

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Abstract

The application of the functional derivatives to the mathematical modeling of complex systems is studied here. The connection of functional derivatives with total differentials in Banach spaces is shown. Local and global existence theorems for the linear equations in total differentials are proved. Consequently, a total integrability conditions are derived for the case of linear equations with the functional derivatives. Some illustrative examples are included.

1. Introduction

The theory of the equations in total differentials in Banach spaces has a long history and this theory occupies a visible place in nearly any textbook devoted to the theory of differential equations (see, e.g., [1–4]). On the contrary, the theory of the equations with functional derivatives is greatly deficient though the application area of that kind of equations is quite broad. Let us mention the area of quantum field theory (e.g., [5–7]), the statistical theory of turbulence (e.g., [8–11]), the area of chemical kinetics (e.g., [12,13]), last but not least, the area of mechanical engineering and numerical mathematics, see, e.g., [14].

Very likely, the reason of the above-mentioned contradiction is that the theory of the equations in total differentials takes independent variables mainly from the n-dimensional Euclidean vector space while the theory of the equations with functional derivatives takes independent variables from functional spaces, making a subsequent analysis incredibly difficult. In fact, only few

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general results were published for the case of rather narrow classes of equations with functional derivatives (see, e.g., [15–18]). The rest of results deals with entirely individualistic types of the equations. The solutions of equations with functional derivatives are sought very often by "trial-and-error" method or some procedures, like the separation of variables or the theory of characteristics. These procedures stem from the theory of ODEs or PDEs.

The functional derivatives have their own remarkable significance relevant to various areas of science and engineering. Let us mention just two of them.

First, the sensitivity theory deals usually with a response of the system solutions to local changes of some parameter(s). The functional derivatives approach allows one to study the sensitivity of the system with respect to whole classes of functions. An application to the reliability analysis can be found in, e.g., [14,19], and the literature cited within there.

Second, the functional derivatives approach lies in the background of a very useful area, namely, in the background of the so-called *density functional theory* (*DFT*). DFT has its origin already in, e.g., [10,11], and the literature quoted within there. It is worth to mention also the following classical source that covers different topics in the statistical mechanics of non-uniform, classical fluids [20]. Today, the DFT has a very broad applications in particle theory, chemical kinetics, quantum chemistry, etc. In the DFT, the functional derivatives form a base when using a variational approach to evaluate the ground state density in multi-particles quantum systems and molecular dynamics. One of the common approaches uses the Kohn–Sham equations facilitating directly the practical calculations. During the recent decades, several DFT theories were developed and adapted to different problems of the multi-particles' theories, see, e.g., [21,22]. The application area is very broad today, see, e.g., [23–28]. The DFT has been also expanded from the stationary case to the time-dependent DFT, as one can found in, e.g., [29,30].

We concentrate ourself to the case of the linear equations with total differentials because the subsequent applications of this linear case is sufficient for our applications. Local and global existence results for the equations in total differentials defined on general Banach spaces will be derived thereby implying the results for the case of the equations with functional derivatives. Finally, the procedure and conditions of derivation of the functional derivatives will be described based on the concept of total differentials.

The rest of the paper is organized as follows. Basic definitions are summarized in Section 2, while Section 3 contains the main results of the paper being the existence results for the equations in total differentials defined on general Banach spaces. Section 4 demonstrates the above-mentioned procedure and conditions for the case of equations with functional derivatives and conditions are shown under which that equations are equivalent to the equations in total differentials. Section 5 gives illustrative examples, while the final section draws some conclusions and gives some outlooks for the future research.

2. Preliminaries

Let us first recall some necessary definitions and facts [31–33]. We suppose that all Banach spaces introduced later on are separable when needed. Let E be a real Banach space and F be a real or complex Banach space. Further, $L(E;F)$ stands for the Banach space of linear bounded mappings with the norm $\|A\| = \sup_{\|x\|=1}\|Ax\|$ and suppose that $U \subset E$ is an open set.

Definition 1. A mapping $f : U \to F$ is called Frèchet differentiable at the point $x \in U$ if there exists a linear bounded operator $A_x \in L(E; F)$ such that

$$\lim_{\Delta x \to 0} \frac{\|f(x+\Delta x) - f(x) - A_x \Delta x\|}{\|\Delta x\|} = 0.$$

The operator A_x is called as the total differential or Frèchet differential at the point $x \in U$. We will denote it as $f'(x)$.

Let the function f be differentiable at all points of the set U, then the mapping $f' : U \to L(E; F)$ is defined. Let the mapping f' be continuous, then the function f is called as continuously differentiable on U, or, as of class C^1. Further, assume that the mapping f' is differentiable on U, then there exists a mapping (the second differential) $f'' = (f')' : U \to L(E; L(E; F))$. The space $L(E; L(E; F))$ is naturally identified with the space $L_2(E; F)$ of bilinear mappings $E \times E \to F$.

Consider a pair of Banach spaces E_1 and E_2 and a mapping $f : E_1 \times E_2 \to F$. The partial differentials are defined as the differentials of the mappings $x_1 \to f(x_1, x_2)$ and $x_2 \to f(x_1, x_2)$. Further consider a functional $\mathcal{F} : C(D) \to \mathbb{R}$, where $C(D)$ is the space of continuous functions, $D \subset \mathbb{R}$ being the domain of their definition. Suppose this functional is Gateaux differentiable at some point $x_0 \in C(D)$ *along* $h \in C(D)$, i.e., its Gateaux derivative

$$\delta\mathcal{F}(x_0; h) = \lim_{\epsilon \to 0} \frac{\mathcal{F}(x_0 + \epsilon h) - \mathcal{F}(x_0)}{\epsilon}$$

exists and it is a continuous linear functional on $C(D)$. Moreover, as a consequence of the Riesz representation theorem there exists a regular countably additive measure μ_{f,x_0} defined on the algebra of closed subsets of D such that

$$\delta\mathcal{F}(x_0; h) = \int_D h(t)\, d\mu_{f,x_0},$$

where $0 < \epsilon \in \mathbb{R}$.

Definition 2. Suppose

$$\delta\mathcal{F}(x_0; h) = \int_D \psi_{\mathcal{F}}(x_0, t) h(t)\, dt,$$

where the function $t \to \psi_{\mathcal{F}}(x_0, t)$ is at least integrable on D. The function $\psi_{\mathcal{F}}(x_0, t)$ is called as the functional derivative of functional $\mathcal{F}$ at the point $x_0 \in C(D)$ and it is denoted as

$$\frac{\delta\mathcal{F}(x_0)}{\delta x(t)}.$$

Definition 3. Suppose $\mathcal{U} = U \times V \subset E \times F$ is an open set in $E \times F$ and $g : \mathcal{U} \to L(E; F)$ is a continuous mapping. Differential equation

$$y' = g(x, y) \tag{1}$$

defines the equation in total differentials for a Frèchet differentiable function y with respect to the independent variable x.

As already noted, let us further restrict ourselves to the case of linear equations, i.e., the function $y \to g(x, y)$ is affine for all $x \in U$. This means that Eq. (1) becomes

$$y' = B(x)y + f(x), \tag{2}$$

where $B : U \to L(F; L(E; F))$ is continuous function, the function f maps U into $L(E; F)$. We suppose that $V = F$. The spaces $L(F; L(E, F))$ and $L(E; L(F, F))$ can be mutually identified and each operator $B \in L(F; L(E; F))$ can be identified with an operator $A \in L(E; L(F; F))$ by the rule $Byh = Ahy$ for every $h \in E$ and $y \in F$. Then, the mapping $B \to A$ defines an isomorphism between Banach spaces $L(F; L(E; F))$ and $L(E; L(F; F))$, moreover, Eq. (2) can be re-written as follows:

$$y'h = A(x)hy + f(x)h \quad \forall h \in E. \tag{3}$$

Definition 4. A solution of Eq. (3) is any single-valued function $y : Q \to F$ of the class C^1, which is defined on the open set $Q \subset U$ and satisfies the equation $y'(x)h = A(x)hy(x) + f(x)h, \ h \in E$ for every $x \in Q$.

Definition 5. Eq. (3) is said to be totally integrable or totally solvable on the open set $U \subset E$, if for arbitrary point $(x_0, y_0) \in U \times F$ there exists a unique solution y of Eq. (3) which is defined in some neighborhood Q of the point x_0 and satisfies the initial condition

$$y(x_0) = y_0. \tag{4}$$

Definition 6. Let $C \in L_2(E; F)$ be an arbitrary bilinear operator. The operation of taking the skewed symmetric part of the bilinear operator C is defined as follows:

$$\bigwedge Chk = \tfrac{1}{2}(Chk - Ckh) \quad \forall h, k \in E. \tag{5}$$

Definition 7. Let L be an arbitrary two-dimensional space in E and let $S(x_0, \ \delta h, \delta k)$ be the triangle in $(x_0 + L) \cap U$ with vertices $x_0, x_0 + \delta h, x_0 + \delta k$, where $h, k \in L$, and with the boundary

$$\Gamma = \overline{x_0\ (x_0 + \delta h)}\ \overline{(x_0 + \delta h)\ (x_0 + \delta k)}\ \overline{(x_0 + \delta k)\ x_0}.$$

The **curl** of a function A at the point $x_0 \in U$ is a bilinear operator **curl** $A(x_0) : E^2 \to L(E; F)$ such that

$$\mathbf{curl}\, A(x_0)hk = \lim_{\delta \to +0} \frac{1}{\delta^2} \int_\Gamma A(s)\, ds \tag{6}$$

uniformly for arbitrary $h, k \in \overline{b(0,1)} \cap L$, where $b(0, 1)$ is the unit ball in E.

Note that if the **curl** exists, then it is uniquely defined and the operator **curl** $A(x_0)$ is skew symmetric.

In the next section, we will need two lemmas (see [31, pp. 170–174]). To formulate these lemmas, let us first introduce some notation. On an oriented closed curve Γ consider the ordering determined by the orientation of p points $x_1, \ldots, x_p$. Further, connect these points to a point x_0 outside Γ or on Γ by means of curves $l_i = x_0 x_i \ \forall \ i = 1, \ldots, p$. The expression $l_i^{-1} = x_i x_0$ stands for the curve reciprocal to l_i. The curves $l_i, l_{i+1}, \ i = 0, 1, 2, \ldots, \mathrm{mod}(p)$ and the arc x_i, x_{i+1} of Γ form a closed curve Γ_i, which can be described as the sequence $x_0 x_i x_{i+1} x_0$ from x_0 to x_0. Then (setting $T_{\Gamma_i} = T_i, P_{\Gamma_i} = P_i$ and $T_{l_i} = T_i$)

$$T_\Gamma = T_l T_p \ldots T_l T_{l^{-1}}.$$

When $T_i = I + P_i$ is introduced, then for $P_\Gamma = T_\Gamma - I$ one obtains the expansion

$$P_\Gamma = T_l \left(\sum_{i=1}^{p} S_i \right) T_{l^{-1}},$$

where $S_i = \sum P_{j_1} \ldots P_{j_i}$ *is taken over all combinations* $p \geq j_1 \geq \cdots \geq j_i \geq 1$. *As the products of the transformations P are in general not commutative the factors in the individual terms of this sum must be taken in the indicated order.*

Lemma 1. *Suppose the operator* $A(x)$ *is continuous in domain U and for each point* $x_0 \in U$ *and for each fixed plane* $L \subset E$ *such that* $x_0 \in L$ *it holds*

$$\lim_{S(x,h,k) \to x_0} \frac{P_\Gamma}{\Delta(x,h,k)} = 0.$$

Here, the triangle $S(x,h,k) = S(x_1,x_2,x_3)$ *with boundary* Γ *in L is meant to converge regularly to* $x_0 \in S$ *while* $\Delta = Dhk$, $h = x_2 - x_1$, $k = x_3 - x_1$ *denotes the real fundamental form of the plane* $S \subset L$ *so that* Δ *represents the oriented area of the triangle. Then the integrability condition* $P_\Gamma = 0$ *holds for every closed, piecewise regular curve in the region U.*

Lemma 2. *Suppose the operator* $A(x)$ *is differentiable at the point* x_0. *Further suppose* $S = S(x_1,x_2,x_3)$ *is a triangle with a boundary* Γ *in a neighborhood containing the point* x_0, δ *is the greatest side length. Then*

$$P_\Gamma = R(x_0)hk + o(\delta^2) = \bigwedge (A'(x_0)hk - A(x_0)hA(x_0)k) + o(\delta^2).$$

Here, for the sake of brevity we put $h = x_2 - x_1, k = x_3 - x_1$.

3. Linear equations in total differentials

In this section, we prove the local existence theory for the homogenous equation (3), i.e., when function $f(x) = 0$. The non-homogenous case will follow as its consequence. After that, we will prove the global existence theorem. First, we formulate the following local existence theorem:

Theorem 1. *Let* $U \subset E$ *be an open set and suppose the function A is differentiable in U. Then the equation*

$$y'h = A(x)hy, \quad h \in E \tag{7}$$

is totally integrable in U if and only if the function $A(x)$ *has the* **curl** *at each point* $x \in U$ *and the equality*

$$\mathbf{curl}\, A(x)hk - \bigwedge A(x)hA(x)k = 0 \quad \forall h,k \in E \tag{8}$$

holds at each point $x \in U$.

Proof. ($\Longrightarrow$). Let $x_0 \in U$, let L be an arbitrary two-dimensional set in E and $h,k \in \overline{b(0,1)} \cap L$. Then, obviously, for $\delta > 0$ small enough, the triangle $S(x_0,\delta h,\delta k)$ lies inside $(x_0 + L) \cap U$ and the function A is (due to its continuity) bounded in some closed ball $\overline{b(x_0,\rho_{x_0})} \subset U$, which contains the triangle $S(x_0,\delta h,\delta k)$. Let on the boundary

$$\Gamma_0 = \overline{x_0(x_0+\delta h)(x_0+\delta k)x_0}$$

of the triangle $S_0(x_0,\delta h,\delta k)$ it holds

$$P_{\Gamma_0} y_0 = \int_{\Gamma_0} A(v)\, dv\, z[v],$$

where z is the solution of Eq. (7) along the curve Γ_0 with the initial condition $z[x_0] = y_0$, $y_0 \in F$. As the function $A(x)$ is differentiable at the point $x_0 \in U$, one can write $A(x) = A(x_0) + A'(x_0)(x - x_0) + o(\|x - x_0\|)$. Moreover, as $z[v] = y_0 + A(x_0)(v - x_0)y_0 + o(\delta)y_0$ with arbitrary y_0,

$$P_{\Gamma_0} = \int_{\Gamma_0} A(v)\,dv + \int_{\Gamma_0} A(x_0)\,dv\,A(x_0)(v-x_0) + \int_{\Gamma_0} [A(v)-A(x_0)]\,dv\,A(x_0)(v-x_0) + o(\delta^2)$$
$$= \int_{\Gamma_0} A(v)\,dv - \bigwedge A(x_0)hA(x_0)k\delta^2 + o(\delta^2). \tag{9}$$

where $\delta = \|x-x_0\|$. Now, using Lemma 1, we have

$$0 = \lim_{\delta\to+0} \frac{P_{\Gamma_0}}{\Delta(x_0,\delta h,\delta k)} = \lim_{\delta\to+0}\frac{P_{\Gamma_0}}{\delta^2} = \lim_{\delta\to+0}\frac{1}{\delta^2}\left(\int_{\Gamma_0} A(v)\,dv - \bigwedge A(x_0)hA(x_0)k\right),$$

which implies that the function A has the **curl** *at the point x_0 and Eq. (8) is granted.*

($\Leftarrow$). Let $x_0 \in U$ be an arbitrary point and let $\rho_{x_0} > 0$ be a real number such that the ball $b(x_0,\rho_{x_0})$ lies entirely inside U including its closure $\overline{b(x_0,\rho_{x_0})}$ and let the function A is bounded on $\overline{b(x_0,\rho_{x_0})}$ (A is differentiable thus continuous on a closed set). Let $L \subset E$ be an arbitrary two-dimensional space and let the set of triangles $S(x,h,k)$ converges to the point x_0 in $(x_0 + L) \cap b(x_0,\rho_{x_0})$ assuming that the point x_0 lies inside each triangle of the set $S(x,h,k)$. As

$$P_\Gamma = \int_\Gamma A(v)\,dv - \bigwedge A(x_0)hA(x_0)k + o(\delta^2),$$

where $\Gamma = \overline{x(x+h)(x+k)x}$, then using of Eq. (8) and of Lemma 2, one gets

$$\lim_{S(x,h,k)\to x_0} \frac{P_\Gamma}{\delta^2} = \lim_{S(x,h,k)\to x_0} \frac{1}{\delta^2}\left(\int_\Gamma A(v)\,dv - \mathbf{curl}\,A(x_0)hk\right) = 0,$$

which, due to Lemma 1, implies the total integrability of Eq. (7). □

The non-homogenous case is solved in the following theorem.

Theorem 2. *Let $U \subset E$ be an open set and suppose the functions $A(x)$, $B(x) \in C^1(U)$. Then the equation*

$$y'h = A(x)hy + B(x)h, \quad h \in E \tag{10}$$

is totally integrable in U if and only if

$$\bigwedge\{A'(x)hk - A(x)hA(x)k\} = 0 \quad \forall h,k \in E \tag{11}$$

$$\bigwedge\{A(x)hB(x)k - B'(x)hk\} = 0 \quad \forall h,k \in E \tag{12}$$

hold at each point $x \in U$.

Proof. The presumptions on the functions $A(x), B(x)$ imply that $y \in C^2(U)$. When differentiating Eq. (10), one gets

$$y''(x)hk = A'(x)khy(x) + A(x)hA(x)ky(x) + A(x)kB(x)h + B'(x)kh.$$

As the mapping $y''(x): E^2 \to F$ is symmetric for each $x \in U$, it follows that the skewed symmetric part

$$\bigwedge\{A'(x)khy + A(x)hA(x)ky + A(x)kA(x)h + B'(x)kh\} = 0$$

for each $h,k \in E$. The above equation is obviously equivalent to the two following equations:

$$\bigwedge\{A'(x)hk - A(x)hA(x)k\} = 0 \quad \forall h,k \in E \tag{13}$$

$$\bigwedge\{A(x)hB(x)k - B'(x)hk\} = 0 \quad \forall h, k \in E \tag{14}$$

for each point $x \in U$. The theorem has been proven. □

Prior to formulate the global existence theorem we introduce the environment we will work in. Let $\mathcal{S}$ be a set of connected subsets of the set U. We introduce, as usual, the ordering on that set by inclusion, i.e., we introduce in $\mathcal{S}$ a structure of the partial ordering according to the rule $S_1 \le S_2$ iff $S_1 \subseteq S_2$. Consider any linearly ordered subset $\mathcal{S}' \subset \mathcal{S}$, such that the union $\bigcup_{S \in \mathcal{S}'} S \subset \mathcal{S}$.

Let us have totally integrable equation

$$y'h = A(x)hy + f(x)h \quad \forall h \in E \tag{15}$$

in an open set $U \subset E$, let the functions $A : U \to L(E; L(E; F))$ and $f : U \to L(E; F)$ be continuous. For arbitrary pair $(x_0, y_0) \in U \times F$ there exists (due to Theorem 1) a solution y, which is defined inside the ball $b(x_0, \rho_{x_0})$ and satisfies the initial condition $y(x_0) = y_0$. We would like to extend the solution y from the ball $b(x_0, \rho_{x_0})$ onto a larger set. As the larger set has to be also the set where, at the same time, the solution is defined, we introduce a pair (y, S), $S \subset U$, defining the solution of Eq. (15). Actually, this solution is given by the open set $S \subset U$ being the definition domain of the solution and of the differentiable function $y : S \to F$ solving Eq. (15).

Definition 8. Let (y, S) be a solution of Eq. (15). An *extension* of that solution is the solution (y_1, S_1) for which $S \subset S_1$ and $y(x) = y_1(x)$ for all $x \in S$.

Definition 9. The solution (y, S) of Eq. (15) is said to be *non-extendable* one in the class $\mathcal{S}$ if for arbitrary extension (y_1, S_1) of that solution with $S_1 \in \mathcal{S}$ it holds that $S_1 = S$.

We formulate now the global existence theorem:

Theorem 3. *Let $(x_0, y_0) \in U \times F$ be an arbitrary point, then there exists a non-extendable solution $(y, S_{x_0 y_0})$ of Eq. (15) in the class $\mathcal{S}$ and $x_0 \in S_{x_0 y_0}$, $y(x_0) = y_0$.*

Proof. Let us define the set

$$\mathcal{S}_{x_0 y_0} = \{S \in \mathcal{S} | x_0 \in S, \exists\ y_S : S \to F,\ (y_S, S) \text{ solves (15) with } y_S(x_0) = y_0\}.$$

On $\mathcal{S}_{x_0 y_0}$ we introduce a partial ordering, which is induced from $\mathcal{S}$, and we will show that each linearly ordered set $\mathcal{S}' \subset \mathcal{S}_{x_0 y_0}$ has a majorant. Let

$$S_0 = \bigcup_{S \in \mathcal{S}'} S. \tag{16}$$

One can see that $x_0 \in S_0$ and $S_0 \in \mathcal{S}$. We define a function $y_{S_0} : S_0 \to F$ as follows: for arbitrary $x \in S_0$ we set $y_{S_0}(x) = y_S(x)$ when $x \in S$. As the set $\mathcal{S}'$ is linearly ordered and the sets $S \in \mathcal{S}$ are connected, the definition of the function y_{S_0} is well posed. Moreover, y_{S_0} satisfies Eq. (15) with the initial condition $y_{S_0}(x_0) = y_0$. Due to Eq. (16) the set S_0 is a majorant for $\mathcal{S}'$. According to the Zorn lemma in the partially ordered set $\mathcal{S}_{x_0 y_0}$ there exists a maximal element, i.e., there exists such $S_{x_0 y_0} \in \mathcal{S}_{x_0 y_0}$ that the inclusion $S_{x_0 y_0} \subset S$, $S \in \mathcal{S}_{x_0 y_0}$ implies that $S = S_{x_0 y_0}$. It means that the solution $(y, S_{x_0 y_0})$ with the definition domain $S_{x_0 y_0}$ is non-extendable in the class $\mathcal{S}_{x_0 y_0}$ and, thus, it is neither extendable in the class $\mathcal{S}$. The proof is completed. □

4. Equations with functional derivatives

The equation with functional derivatives with respect to an unknown functional y is the following relation:

$$\frac{\delta y(x)}{\delta x(t)} = g(x, t, y(x)). \tag{17}$$

The right-hand side of Eq. (17) represents a function, which is defined on $U \times D \times \mathbb{R}$, where U is an open set in $C(D)$. We suppose that this function is continuous on $U \times D \times \mathbb{R}$.

By a solution of Eq. (17) we mean every functional $y : S \to \mathbb{R}$, which is defined on an open set $S \subset U$ and satisfies on that set the relation (17) for every $t \in D$. Eq. (17) is said to be totally integrable if for each pair $(x_0, y_0) \in U \times \mathbb{R}$ there exists a unique solution of that equation with the initial condition $y(x_0) = y_0$.

As the function g is continuous (see the definition of functional derivative), Eq. (17) is equivalent to the following equation in total differentials:

$$y'h = P(x, y)h, \quad h \in C(D), \tag{18}$$

where y' is the Frèchet differential of the functional y and

$$P(x, y)h = \int_D g(x, t, y)h(t)\, dt$$

for each $h \in C(D)$.

As a result, we can formulate the following theorem:

Theorem 4. *Suppose we have the following equation in functional derivatives*

$$\frac{\delta y(x)}{\delta x(t)} = g(x, t, y(x)), \tag{19}$$

where the function $g(x, t, y(x))$ *is supposed continuous on* $U \times D \times \mathbf{R}$, D *is supposed to be compact and* $y(x)$ *is a functional. Then Eq. (19) is equivalent to the equation in total differential*

$$y'h = P(x, y)h, \quad h \in C(D), \tag{20}$$

where y' *is the Frèchet differential of the functional* y *and*

$$P(x, y)h = \int_D g(x, t, y)h(t)\, dt$$

for every $h \in C(D)$. *The equivalence is meant in the sense that every solution of Eq. (19) is the solution of Eq. (20) and vice versa.*

Proof. We take the functional derivative as a function of two variables x, t. As that function is continuous in both variables, then, due to compactness of the set D, the continuity of the mapping

$$x \to \frac{\delta y(x)}{\delta x(t)}$$

is uniform with respect to $t \in D$. That means that for all $\epsilon > 0$ there exists $\delta > 0$ such that when $\|x_1 - x_2\| < \delta$ then

$$\left| \frac{\delta y(x_1)}{\delta x(t)} - \frac{\delta y(x_2)}{\delta x(t)} \right| < \epsilon$$

for each $t \in D$. It immediately implies that the mapping

$$h \to \int_D \frac{\delta y(x)}{\delta x(t)} h(t)\, dt = \delta y(x; h) \in \mathbf{R}, \quad h \in C(D) \tag{21}$$

defines the Frèchet differential y' of the functional y. As the function G is continuous, then due to Eq. (21), Eq. (19) is equivalent to Eq. (20) where $P(x,y)h = \int_D g(x,t,y)h(t)\, dt$ for every $h \in C(D)$. The theorem is proven. □

Thus, the problem of the analysis of the equations with functional derivatives is transformed into the problem for the equations in total differentials. As we mentioned already, we target the linear equations with functional derivatives. So, we will analyze the linear equation in functional derivatives

$$\frac{\delta y(x)}{\delta x(t)} = a(x,t)y(x) + b(x,t) \tag{22}$$

and we suppose that the functions $a: U \times D \to \mathbb{R}$, $b: U \times D \to \mathbb{R}$ are continuous. Denote

$$A(x)h = \int_D a(x,t)h(t)\, dt, \quad B(x)h = \int_D b(x,t)h(t)\, dt, \ h \in C(D). \tag{23}$$

Using Eq. (23), Eq. (22) can be re-written as the following equation in total differentials:

$$y'h = A(x)hy + B(x)h, \quad h \in E = C(D) \tag{24}$$

with continuous functions $A: U \to C(D)$, $B: U \to C(D)$.

Now, we can apply the results of the previous section to Eq. (24) to obtain the following:

Theorem 5. *Suppose the functions a, b have continuous functional derivatives in $U \times D$ with respect to x. Then Eq. (22) is totally integrable if and only if the following relations are satisfied:*

$$\frac{\delta a(x,t)}{\delta x(s)} = \frac{\delta a(x,s)}{\delta x(t)}, \tag{25}$$

$$\frac{\delta b(x,t)}{\delta x(s)} + a(x,s)b(x,t) = \frac{\delta b(x,s)}{\delta x(t)} + a(x,t)b(x,s) \tag{26}$$

for each $x \in U$ and each $s, t \in D$.

Proof. Theorem 2 implies that Eq. (24) and thus the equivalent equation (22) are totally integrable if and only if the following relations are valid:

$$A'(x)hk = A'(x)kh, \tag{27}$$

$$\bigwedge \{A(x)hB(x)k - B'(x)hk\} = 0 \tag{28}$$

for arbitrary $h, k \in C(D)$. Since

$$A'(x)hk = \int_D \int_D \frac{\delta a(x,t)}{\delta x(s)} h(s)k(t)\, ds\, dt,$$

it follows that Eq. (27) is equivalent to the relation (25). Similarly, Eq. (28) is equivalent to the relation (26). The theorem has been proven. □

5. Examples

In this section, the following examples to illustrate the previous results are given.

Example 1. The Schrödinger equation in functional derivatives [5] is often used in the quantum field theory. It has the following form:

$$i\frac{\delta y(x)}{\delta x(t)} = H(t,x), \tag{29}$$

where $y(x) = S(x)\Phi$, Φ is a constant, $S(x)$ is the scattering matrix of interaction with an intensity x; $y(x)$ is the amplitude of the system state. The operator $H(t,x)$ is a generalized Hamiltonian and it is calculated via scattering matrix. The conditions of total integrability are expressed by

$$\frac{\delta H(t,x)}{\delta x(s)} = \frac{\delta H(s,x)}{\delta x(t)}.$$

The solutions of that equation are expressed in the form

$$y(x) = y_0 + \int_{x_0}^{x} H(t,v)\,\delta v, \quad y(x_0) = y_0.$$

Example 2. Next example, see [34], follows from the Schwinger equation, when the Fourier transformation is applied

$$\frac{\delta G(x,\xi)}{\delta x(t)} = \left[\frac{\delta \ln \Phi(x)}{\delta x(t)} - \frac{i}{a^2}(-|\xi|^2 + a^2)\right] G(x,\xi), \tag{30}$$

where Φ is known characteristic functional of a random quantity, a is a positive constant, $\xi = (\xi_1, \xi_2, \xi_3) \in \mathbf{R}^3$, $\xi^2 = \xi_1^2 + \xi_2^2 + \xi_3^2$, $x \in C(D)$ is an element of the space $C(D)$, $D \subset \mathbf{R}^3$, of real continuous functions, and $G : C(D) \times \mathbf{R}^3 \to (R)$ is the unknown function. Eq. (30) plays an important role in the theoretical physics, see [34].

Supposing that the function Φ is sufficiently smooth, we can apply Theorem 5. As a result, Eq. (30) is totally integrable and the solution set is done by

$$G(x,\xi) = \exp\left\{-\int_0^x \left[\frac{\delta \ln \Phi(v)}{\delta v(t)} - \frac{i}{a^2}(|\xi|^2 - a^2)\right]\delta v\right\} q(\xi), \tag{31}$$

where $q(\xi) = G(0,\xi)$ is the initial function. The functional integral (31) can be easily evaluated. As a result, the function G takes the form

$$G(x,\xi) = \frac{1}{\Phi(x)} \exp\left\{\frac{i}{a^2}(|\xi|^2 - a^2)\int_D x(t)\,dt\right\} q(\xi).$$

6. Conclusion and outlooks

The connection between total differentials and functional derivatives has been used to analyze the linear equations with first-order functional derivatives, very often used in different areas of physics, chemistry and engineering. Conditions when the solution of such equations exists were derived.

The area of equations with functional derivatives is still open and the results are mostly based on some amount of erudition. The general theory of solutions of differential equations with functional derivatives is still missing though some primary results can be found mostly in the area of quantum field theory models. Nevertheless, the problems are generally processed on the case-by-case basis.

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