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MODELLING DELAYED SIGNALS IN BIOLOGICAL SAMPLES

Mihaela Ghelmez (Dumitru), Cristian Toma, Silviu-Mihai Tanase,
Ciprian Cojocarasu, Paul Constantinescu
Politehnica University Bucharest, mghelmez@yahoo.com

Abstract: *We consider a function similar to a spline function, and a system described by a differential equation of evolution, with a free term corresponding to an external pulse. Its simulation, performed in Matlab, is suitable for modeling delayed pulses.*
It results that this type of differential equation, working on limited time interval, is suitable for modeling pulses which present a minimum negative value before starting to rise towards a final positive value. The presence of fluctuations was taken into account, too.
This behavior is appropriate for some liquid crystal fatty acids samples, in interaction with laser fields, presented in the paper.
Keywords*: spline function, delayed pulses, differential equations, liquid crystals, fatty acids, laser fields*

1. INTRODUCTION

Many complex molecular structures of the living matter pass through a mesomorphic state, which is involved in explaining their evolution during the interaction with some external stimuli [1, 2]. The liquid crystal state of some fatty acids (FA) and FA mixtures with cholesterol (Ch) was experimentally studied, taking into account their role in humans, animals and plants. The possibility of inducing a non-linearity in such systems could lead to a radical change of their dynamics. Experimental and theoretical studies performed in our laboratory [3] and in co-operation with other research sites showed that, in different nonlinear optical media, interesting answers were obtained when a laser beam passed through the substance. Consequently, some mathematical formalism was developed for describing this answer, and different computer facilities were used for data processing and for some mathematical models building.

2. MATERIALS AND METHODS

This paper presents a study of some components or forerunners of the biological membrane, namely: (BA) butyric acid $CH_3CH_2CH_2COOH$: (LA) lauric acid $CH_3(CH_2)_{10}COOH$; (AA) arachidonic acid (all-cis-5,8,11,14-eicosatetraenoic), or FA and Ch ($C_{27}H_{45}OH$) mixtures in different molar percentages. At the polarizing microscope, FA and their mixtures with Ch or other substances showed a smectic liquid crystal SLC texture during the evolution between some temperature values [3].

These FA were encapsulated in our laboratory at “Politehnica” University, by melt drawing into 25µm thickness cells with transparent flat electrodes of SnO_2.

The computer programs were written in MATLAB software. They were applied to study the special non-linear behavior of our mesomorphic systems while in a radiation field. The Gaussian form of the beam was studied before and after passing through the samples. An example of the obtained experimental data are presented in Figure 1 a, b, for the pure BA and the mixture BA-Ch 2÷1. These data were measured with an experimental setup presented in [4] and containing a He-Ne 6328Å and 20mW power laser, focused on a sandwiched liquid crystal cell with FA and, respectively, with mixtures.

A focusing lens has been placed between the laser and the sample and a detection stage completed the installation, comprising a photoresistive detector, that can be displaced both on x and y axes and a measuring stage for the emergent voltage, monitored by the detector with the help of a resistor. This is a measure of the laser emergent intensity and the spatial extension of the beam can be displayed. The experimental results were processed with the Table Curve3D program. By checking all the fitting equations we could state that the Gaussian form is better preserved by mixture samples than the pure ones. The program gives other useful information on the experimental data, and therefore one can also choose other experimental conditions in terms of the future experiment requirements and purpose.

A strong spread of the He-Ne laser light was observed in LA and LA-Ch samples. A refractive index modification with the cholesterol percentage or at the interaction with the light field seems to appear in all the samples. The large change of the refractive index with the light intensity leads to the possibility of the self-focusing of the laser beam in

AA and other effects - such as the optical activity nonlinear change [5] with the intensity of the light in LA and mixtures with Ch. Also the laser pulse width modification after passing through all the samples was observed and correlated with the Ch percentage. One can see the pulses shape in LA and mixtures in Figure 2 and the pulses width in terms of the Ch percentage and applied voltage in AA and mixtures in Figure 3.

Using an Nd^{3+} glass laser has emphasized the pulse width modification in time domain, according to [6]. A KDP crystal has been used for obtaining a visible light at 523nm, and the output features were displayed on a sampling oscilloscope at 0.05 V/div. One can see the effect of the Ch amount in mixtures of FA, which can develop a method to estimate this amount by means of the output pulse width.

3. ASPECTS REGARDING POSSIBILITIES OF USING SPLINE FUNCTIONS FOR MODELING DELAYED PULSES AND PULSES PRESENTING A MINIMUM VALUE DURING TRANSIENT REGIME

We consider the function

$$f(t) = (t-1)^2 tx+1)^2 \qquad (1)$$

similar to a spline function, with null values for f(t) and for its first derivative for t= -1 and for t = 1.
Its first derivative is

$$f'(t) = 4t^3-4t \qquad (2)$$

and its second derivative:

$$f''(t) = 12t^2-4 \qquad (3)$$

This allows us to write the equation

$$f''(t) = -6f(t) + 6t^4 -4 \qquad (4)$$

which can be defined on the time interval (-1, 1) from initial null conditions. It results a pulse having the maximum value equal to unity.

A) Let us now consider a system described by the differential equation of evolution presented above, with a free term corresponding to an external pulse with amplitude equal to 10 multiplied by a function $1/(t-1)^4$ (applied at a time moment close to t = -1). It results the equation

$$f^{(2)}(t) = -6\, f(t) + 6t^4 -+2 +10/(t-1)^4 \qquad (5)$$

starting to work from initial null conditions form a certain time moment very close to t = -1 (t= - 0.99). Its simulation (performed in Matlab) has generated the function presented in figure 4. It can be noticed that the function f presents a significant variation after the time moment t= 1.5, of about three quarters of the whole working interval (-1, 1). This shows that this type of differential equation is suitable for modeling delayed pulses.

B). Let us now consider a system described by the differential equation of evolution presented above, with a free term corresponding to an external pulse with amplitude equal to 10 multiplied by a function $1/(t^4-1)$ (applied at a time moment close to t = -1). It results the equation

$$f^{(2)}(t) = -6\, f(t) + 6t^4 -+2 +10/(t^4 -1) \qquad (6)$$

starting to work from initial null conditions form a certain time moment very close to t = -1 (t= - 0.99). Its simulation (performed in Matlab) has generated the function presented in figure 5. It can be noticed that the function f presents a significant minimum negative value, before starting to rise towards a final value, when t is close to 1 and the first order derivative f'(t) is close to zero. Moreover, the module of this final value is less than the module of the minimum negative value. It results that this type of differential equation, working on a limited time interval, is suitable for modeling pulses which present a minimum negative value before starting to rise towards a final positive value.

4. ANALYSIS OF FLUCTUATIONS

Since the investigated structures are very sensitive at random variations of the integration period (generated by the switching phenomena at the end of the integration) a multiplication of the received signal with a test-function is recommended. We present some invariance properties of differential equations, which can be used for generating a "practical" test-function on this time interval. We were looking for "truncated" test functions and presenting the properties of a second order oscillating systems, considered as generating "practical" test functions, in filtering and sampling procedures. Numerical simulations were using Runge-Kutta equations of order 4-5 in MATLAB. TableCurve3D program was used to fit the experimental dependencies of the output signals on different input physical amounts. A good agreement between the experiment and computer results was found. A method to estimate the cholesterol percentage in a mixture with fatty acids was developed.

For taking into account the fluctuations we begin our analysis by writing a test function similar to a Dirac pulse under the form:

$$\varphi = \exp\,[1/(\tau^2 - 1)] \qquad (7)$$

where $\tau = t - t_{sym}$, t_{sym} being the middle of the working period. Such a function has nonzero values only for $\tau \in [-1, 1]$. The derivatives $\varphi^{(1)}$, $\varphi^{(2)}$ and $\varphi^{(3)}$ of this function as related to τ are:

$$\varphi^{(1)} = [-2\tau/(\tau^2-1)^2]\, \exp[1/(\tau^2-1)] \qquad (8)$$

$$\varphi^{(2)} = [(6\tau^4 - 2) / (\tau^2-1)^2] \exp[1/(\tau^2-1)] \qquad (9)$$
$$\varphi^{(3)} = [(24\tau^7 - 60\tau^5 + 24\tau^3 + 4\tau) / (\tau^2-1)^2] \exp[1/(\tau^2-1)] \qquad (10)$$

We are looking for a differential equation, which can have as a solution the function φ. Such an equation cannot generate the test function φ. The existence of such an equation of evolution, beginning to act at an initial moment of time, would imply the necessity for a derivative of certain order n - noted $f^{(n)}$ - to make a "jump" at this initial moment from the "zero" value to another value which differs to zero. Such an aspect would be in contradiction with the property of the test-functions to have continuous derivatives of any order on the whole real axis, represented in this case by the time axis. It results that an ideal test-function could not be generated by a differential equation, but it is quite possible for such an equation to possess as a solution a "practical" test function f, i.e. a function with nonzero values on the interval $\tau \in [-1, 1]$ and a certain number of continuous derivatives on the whole time axis. Therefore we will try to study such evolutions depending only of the values f, $f^{(1)}$,$f^{(n)}$, these values being equal to the values of φ, $\varphi^{(1)}$, ..$\varphi^{(n)}$ at a certain time moment, very close to the initial moment τ = -1. Taking into account the expressions of φ, $\varphi^{(1)}$, the simplest differential equation satisfying these requirements, has the form:

$$f^{(1)} = [-2\tau/(\tau^2 - 1)] f \qquad (11)$$

and has the function φ as a possible solution. As an initial moment of time we chose τ_0 = -1 + 0.01 and as an initial condition for f we chose the value $\varphi(\tau_0)$. By numerical simulation using equations Runge-Kutta of 4-5 order in MATLAB it has been obtained as solution a function f having a form similar to φ, but with very small amplitude of about 10^{-12}.

We can continue the analysis by studying a second order differential equation without "free" term, which has as possible solution the function φ. Taking into account the expressions of φ, $\varphi^{(2)}$, such an equation could be:

$$f^{(2)} = [(6\tau^4 - 2)/(\tau^2 - 1)] f \qquad (12)$$

As initial conditions for f, $f^{(1)}$ we chose the values of φ, $\varphi^{(1)}$ at the time moment τ_0 = -1 + 0.01. The numerical simulation (using the same Runge-Kutta functions in MATLAB) presents as solution a function with a form similar to φ, but still with small amplitude. (The amplitude is only four times greater than the amplitude obtained for a first order differential equation.

Let us try now to obtain a function similar to a rectangular unity pulse. For this purpose, we consider a test function having the form:

$$\varphi_a = \exp[0.1/(\tau^2-1)] \qquad (13)$$

We are using a second order differential equation (without "free" term) under the form:

$$f^{(2)}(\tau) = [(0.6\tau^4 - 0.36\tau^2 - 0.2)/(\tau^2-1)^4] f(\tau) \qquad (14)$$

suggested by the expressions of φ_a, $\varphi_a^{(2)}$), and with initial conditions for f, $f^{(1)}$ equal to 0.0002 and 0.02 respectively, at the initial time moment τ = -1 + 0.01. One obtains as solution, using the same Runge-Kutta functions in MATLAB, a function very close to a rectangular unitary pulse; the amplitude is close to unity for more than 2/3 of the integration period.

For processing a laser signal emergent from the medium we must consider null initial conditions for the system, and we must also add a "free" term in the differential equation – corresponding to the laser pulse emergent from the material. The working period was chosen about 10 times greater than the pulse width, considered to have a Gaussian form. The time interval between the beginning of the working period and the moment of time corresponding to the maximum of the Gaussian pulse with the simplest form of $A \exp(-(\tau-\tau_0)^2/\sigma^2)$ has been considered equal to 10σ. This means that the oscillating system was activated by the front of the received Gaussian pulse. Under these circumstances, the differential equation must be written as

$$f^{(2)} = ((0.6\tau^4 - 0.36\tau^2 - 0.2)/(\tau^2 - 1)^4) f + A \exp(-(\tau+0.9)^2/(0.01)^2) \qquad (15)$$

By numerical simulations in MATLAB with Runge-Kutta functions we have obtained the results presented in Figure 6. It can be easily noticed that from an emergent pulse width less than 0.1, another pulse having the width of 2 units (more than an order of magnitude longer than the received pulse) has been obtained. So this function f, generated by the processing system, can be easily integrated, due to the time interval on which it differs to zero, the working speed of the electronic devices being high enough for processing such a "longer" signal. Two aspects must be also noticed:

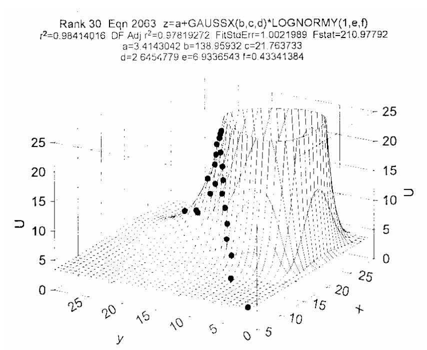
a) at the end of the integrating period (when τ = 1) the integrated signal - the function f - has a value of about 10% from the peak obtained on the time interval (-1, 1), and therefore the system is also robust at the fluctuations of the integrating period;
b) the result obtained for the function f generated by the processing system is proportional to the amplitude A of the Gaussian laser pulse emergent from the material – as has been noticed by using numerical simulations in MATLAB with A = 1, A = 0.1 and A = 0.001. Thus the result of the integration is also proportional to the amplitude of the laser pulse.

5. CONCLUSIONS

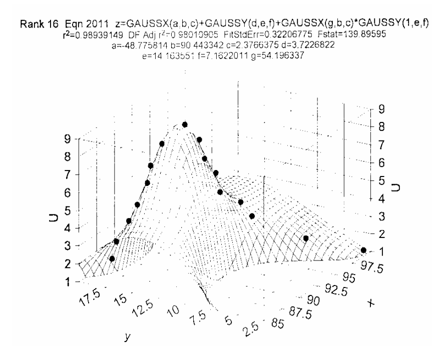
As it is known, in averaging procedures the user is interested in the mean value of the received signal over a certain time interval. Since the investigated structures are very sensitive at random variations of the integration period (generated by the switching phenomena at the end of the integration) a multiplication of the received signal with a test-function is recommended. We consider a function similar to a spline function, and a system described by a differential equation of evolution, with a free term corresponding to an external pulse. Its simulation, performed in Matlab, is suitable for modeling delayed pulses.

In the paper we presented also some invariance properties of differential equations, which can be used for generating a "practical" test-function on this time interval. We were looking for "truncated" test functions (functions which differ to zero only on a certain interval and with only some derivatives continuous on the real axis) and we presents also the properties of second order oscillating systems (considered as generating "practical" test functions) in filtering and sampling procedures [7]. Numerical simulations were using Runge-Kutta equations of order 4-5 in MATLAB. TableCurve3D program was used to fit the experimental dependencies of the output signals on different input physical amounts. A good agreement between the experiment and computer results was found. A method to estimate the cholesterol percentage in a mixture with fatty acids was developed.

Since fatty acids and cholesterol are important substances for the living matter and especially for the biological membrane [8], we consider this study important for elucidating some mechanism belonging to this domain. and a promising bridge to biophysical studies by the non-linear dynamics methods.



a)



b)

Figure 1a, b Laser emergent beam from: a) the pure butyric acid sample; b) mixture sample. U-emergent voltage; x, y, -horizontal and vertical co-ordinates of the detector.

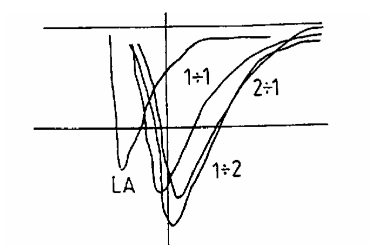


Figure 2 Nd^{3+}laser pulse emergent from samples of LA and mixtures with Ch

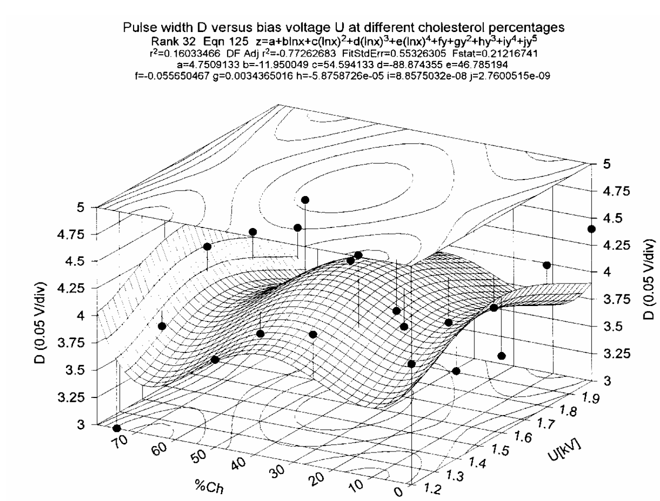


Figure 3.

Pulse width D versus bias voltage U at different Ch percentage. Nd^{3+} glass laser SOLARS S-7, IFTAR Bucharest, TEM_{002} , 200 µs, 1.06 µm (SHG 532 nm); sampling oscilloscope TEKTRONIX 7613 (0.05V/div. and 0.5 ms/div.)

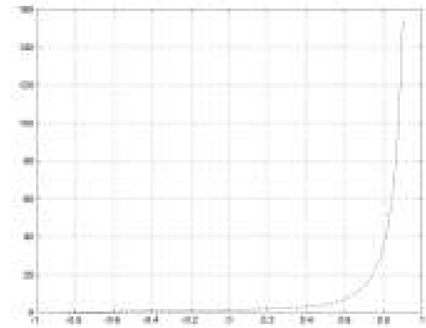


Figure 4 Figure 4. Spline delayed function

Figure 5. Spline reversed function

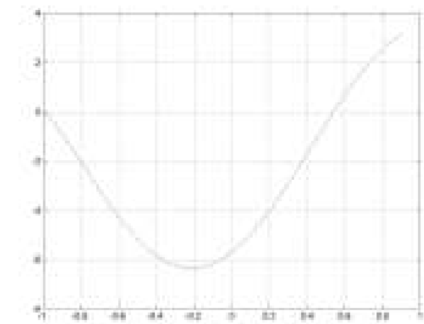


Figure 6. Theoretical emergent laser signal intensity versus time in presence of fluctuations

REFERENCES

[1] I.C.Khoo, Y.R.Shen*,* Optical Engin., 24, pp.4-25, 1985

[2] M..Dumitru (Ghelmez), M. Honciuc, M.C.Piscureanu, C.Gheorghe, "New Nonlinear Optical Materials for Optoelectronics", *Optical Engin*. 35(5), pp.1372-1376, 1996

[3] M..Dumitru (Ghelmez), M.Honciuc, I. Craita, "Nonlinear Optical Effects in Fatty Acids Complex Systems"*,* The VIth Intl. Congress of the European Medical Association (EMLA'98), 3-5 June 1998, Bucharest, Romania*, EMLA J. of Telematics*, Nr.1, 1999

[4] M. Ghelmez (Dumitru), M.Honciuc, E.Slavnicu, B.Dumitru, R.I.Trascu, "Laser study of the butyric acid and some mixtures", *Rom.J.Optoelectronics,* 9, 1, pp. 3-13, 2001

[5] M.Dumitru (Ghelmez), M.Honciuc, I.M.Popescu, "Interaction of some laser radiation with the lauric acid in mesophase", SPIE Vol.2138, pp.148-155, 1994

[6] A. Adolf, D. Chatrefou, and C. Guedard, "Elargissement du spectre temporel et spatial dans un milieu optique non lineaire. Etude d'un oscillateur bimode", *J.Opt.(Paris),* Vol15, No.2, 83-93, (1984)

[7] S.Gong,H.Hentzell,S.Peterson,H.Hesselbon,B.Lofstedt,M.Hause,"Techniques for Reducing Switching Noise in High-Speed Digital Systems" –Proc. 8th Annual Intl. ASIC Conference, 18-21 Sept. 1995

[8] M. Dumitru, "Operating conditions of some liquid crystals in interaction with physical fields", in *Liquid Crystals:Chemistry and Structure,* M.Tykarska, R.Dabrowski, J.Zielinski, Editors, Proceedings of SPIE Vol. 3319, 326-333 (1998)