

# Polymer Dynamics Through Group Invariance of $SL(2R)$ – Type in a Fractal Paradigm

CONSTANTIN PLACINTA<sup>1</sup>, TUDOR CRISTIAN PETRESCU<sup>2</sup>, VLAD GHIZDOVAT<sup>3</sup>,  
STEFAN ANDREI IRIMICIUC<sup>4</sup>, DECEBAL VASINCU<sup>5</sup>, MARICEL AGOP<sup>6,7</sup>,  
VIOREL-PIIU PAUN<sup>8\*</sup>

<sup>1</sup>Materials Science Department, Gheorghe Asachi Technical University, 59A Prof. dr. docent Dimitrie Mangeron Blvd., 700050, Iasi, Romania

<sup>2</sup>Department of Structural Mechanics, “Gheorghe Asachi” Technical University, 1Prof. dr. docent Dimitrie Mangeron Blvd., 700050, Iasi, Romania

<sup>3</sup>Grigore T. Popa University of Medicine and Pharmacy, Faculty of Medicine, Biophysics and Medical Physics Department, 16 University Str., 700115, Iasi, Romania

<sup>4</sup>National Institute for Laser, Plasma and Radiation Physics, 409 Atomistilor Str., 077125, Bucharest, Romania

<sup>5</sup>Grigore T. Popa University of Medicine and Pharmacy, Faculty of Dental Medicine, Biophysics and Medical Physics Department, 16 University Str., 700115, Iasi, Romania

<sup>6</sup>Physics Department, Gheorghe Asachi Technical University, 59A Prof. dr. docent Dimitrie Mangeron Blvd., 700050, Iasi, Romania

<sup>7</sup>Academy of Romanian Sciences, 54 Splaiul Independentei, 050094, Bucharest, Romania

<sup>8</sup>University Politehnica of Bucharest, Faculty of Applied Sciences, Physics Department, 313 Splaiul Independentei, 060042, Bucharest, Romania

**Abstract.** *We analyze polymer dynamics in a fractal paradigm. Then, it is shown that polymer dynamics in the form of Schrödinger – type regimes imply synchronization processes of the polymers’ structural units, through joint invariant function of two simultaneous isomorphic groups of  $SL(2R)$  – type, as solutions of Stoka equations. In this context, period doubling, damped oscillations, self – modulation and chaotic regimes emerge as natural behaviors in the polymer dynamics. The present model can also be applied to a large class of materials, such as biomaterials, biocomposites and other advanced materials.*

**Keywords:** *fractal paradigm, polymers, Schrödinger – type regimes, joint invariant function, isomorphic groups*

## 1. Introduction

To describe polymer dynamics in the fractal paradigm, but remaining faithful to the differentiable mathematical procedures, it is necessary to explicitly introduce scale resolutions, both in the expression of the variables and in the fundamental equations which govern polymer dynamics. This means that, instead of “working” with a single variable described by a strict non-differentiable function, it is possible to “work” only with approximations of these mathematical functions obtained by averaging them on different scale resolutions. As a consequence, any variable purposed to describe polymer dynamics will perform as the limit of a family of mathematical functions, this being non – differentiable for null scale resolutions and differentiable otherwise [1, 2].

In the present paper, considering the fractal paradigm as being functional [1-4], a non – differentiable model describing various polymer dynamics is proposed.

## 2. Theoretical part

### 1. Mathematical Model

The polymer is a set of entities (or structural units) that, through their interactions, relationships or dependencies form a unified whole.

\*email: [viorel.paun@physics.pub.ro](mailto:viorel.paun@physics.pub.ro), [viorel\\_paun2006@yahoo.com](mailto:viorel_paun2006@yahoo.com)

All authors have contributed equally to this paper.



In what follows, the polymer will be assimilated with a fractal. Such an assumption is sustained by the following example, related to the collision processes in a polymer: between two successive interactions (collisions) of structural units, the trajectory of the entity is a straight line that becomes non – differentiable in the impact point. Considering that all the collision impact points form an uncountable set of points, it results that the trajectories of the polymer structural units become continuous and non – differentiable curves, i.e. fractal curves. In such a context, the Fractal Theory of Motion in the form of Scale Relativity becomes operational through the scale covariant derivative [3, 4]:

$$\frac{\hat{d}}{dt} = \partial_t + \hat{V}^l \partial_l + \frac{1}{4} (dt)^{\left(\frac{2}{D_f}\right)-1} D^{lp} \partial_l \partial_p, \tag{1}$$

where

$$\begin{aligned} \hat{V}^l &= V_D^l - V_F^l \\ D^{lp} &= d^{lp} - i \hat{d}^{lp} \\ d^{lp} &= \lambda_+^l \lambda_+^p - \lambda_-^l \lambda_-^p \\ \hat{d}^{lp} &= \lambda_+^l \lambda_+^p + \lambda_-^l \lambda_-^p \\ \partial_t &= \frac{\partial}{\partial t}, \partial_l = \frac{\partial}{\partial x^l}, \partial_l \partial_p = \frac{\partial}{\partial x^l} \frac{\partial}{\partial x^p}, i = \sqrt{-1}, l, p = 1, 2, 3 \end{aligned} \tag{2}$$

In the above – written relations,  $x^l$  is the fractal spatial coordinate,  $t$  is the non – fractal time having the role of an affine parameter of the motion curves,  $\hat{V}^l$  is the complex velocity,  $V_D^l$  is the differential velocity independent on the scale resolution  $dt$ ,  $V_F^l$  is the non – differentiable velocity dependent on the scale resolution,  $D_F$  is the fractal dimension of the movement curve,  $D^{lp}$  is the constant tensor associated with the differentiable – non – differentiable transition,  $\lambda_+^l (\lambda_+^p)$  is the constant vector associated with the backward differentiable – non – differentiable physical processes and  $\lambda_-^l (\lambda_-^p)$  is the constant vector associated with the forward differentiable – non – differentiable physical processes. Fractal dimensions can be defined in more than one way: more precisely, the fractal dimension in the sense of Kolmogorov, the fractal dimension in the sense of Hausdorff – Besikovitch etc. [2, 5, 6]. Selecting one of these definitions and operating it in the polymer dynamics, the value of the fractal dimension must be constant and arbitrary for the entirety of the dynamical analysis: for example, it is regularly found  $D_F < 2$  for correlative processes,  $D_F > 2$  for non – correlative processes, etc. [1, 5, 6].

Now, accepting the functionality of the scale covariance principle i.e. applying the operator (1) to the complex velocity field from (2), in the absence of any external constraint, the motion equation of the polymer structural units (i.e. the geodesics equation on a fractal space) takes the following form [3, 4]:

$$\frac{\hat{d}\hat{V}^i}{dt} = \partial_t \hat{V}^i + \hat{V}^l \partial_l \hat{V}^i + \frac{1}{4} (dt)^{\left(\frac{2}{D_f}\right)-1} D^{lk} \partial_l \partial_k \hat{V}^i = 0, \tag{3}$$

This means that the fractal acceleration  $\partial_t \hat{V}^i$ , the fractal convection  $\hat{V}^l \partial_l \hat{V}^i$  and the fractal dissipation  $D^{lk} \partial_l \partial_k \hat{V}^i$  in the polymer structural units' dynamics, are in equilibrium in any point of the fractal curve.

If the fractalisation is achieved by Markov – type stochastic processes [2, 5, 6], then:

$$\lambda_+^i \lambda_+^i = \lambda_-^i \lambda_-^i = 2\lambda \delta^{ii}, \tag{4}$$

where  $\lambda$  is a coefficient associated to the differentiable – non – differentiable transition and  $\delta^{ii}$  is Kronecker's pseudo – tensor.

Under these conditions, the geodesics equation (3) takes the simple form:

|  |     |
|--|-----|
| $\frac{d\hat{V}^i}{dt} = \partial_t \hat{V}^i + \hat{V}^l \partial_l \hat{V}^i - i\lambda(dt)^{\left(\frac{2}{D_f}\right)^{-1}} \partial^l \partial_l \hat{V}^i = 0$ | (5) |
|--|-----|

2. Dynamics of polymers structural units in the form of Schrodinger – type “regimes”

For irrotational motions of the polymer structural units, the complex velocity field  $\hat{V}^i$  from (2) takes the form:

|  |     |
|--|-----|
| $\hat{V}^i = -2i\lambda(dt)^{\left(\frac{2}{D_f}\right)^{-1}} \partial^i \ln \Psi$ | (6) |
|--|-----|

where  $\ln \Psi$  is the fractal scalar potential of the velocity fields and  $\Psi$  is the state function.

Then, substituting (6) in (5) the geodesics equation (5) becomes (for details on the method, [3, 4].

|   |     |
|---|-----|
| $\lambda^2(dt)^{\left(\frac{4}{D_f}\right)^{-2}} \partial^l \partial_l \Psi + i\lambda(dt)^{\left(\frac{2}{D_f}\right)^{-1}} \partial_t \Psi = 0$ | (7) |
|---|-----|

This is a Schrödinger equation of fractal type. Therefore, various dynamics of any polymer structural units can be implemented as Schrödinger – type fractal “regimes” (i.e. at various scale resolutions).

In the one – dimensional stationary case, the Schrödinger equation of fractal type takes the form (for details on the method see [1, 3, 4]):

|  |     |
|--|-----|
| $\frac{d^2 \Psi}{dx^2} + k_0^2 \Psi = 0$ | (8) |
|--|-----|

with

|   |     |
|---|-----|
| $k_0^2 = \frac{E}{2m_0 \lambda^2 (dt)^{\left(\frac{4}{D_f}\right)^{-2}}}$ | (9) |
|---|-----|

In (8)  $x$  is the fractal spatial coordinate,  $E$  is the fractal energy of the polymer entity and  $m_0$  is the rest mass of the polymer entity.

In the general case,  $\Psi(x)$  is a complex function. Considering that,  $\Psi(x)$  can be written in the form:

|                          |      |
|--------------------------|------|
| $\Psi(x) = X(x) + iY(x)$ | (10) |
|--------------------------|------|

so that Eq. (8) in real variables becomes:

|                                    |      |
|------------------------------------|------|
| $\frac{d^2 X}{dx^2} + k_0^2 X = 0$ | (11) |
|------------------------------------|------|

|                                    |      |
|------------------------------------|------|
| $\frac{d^2 Y}{dx^2} + k_0^2 Y = 0$ | (12) |
|------------------------------------|------|

Relations (11) and (22) are invariant to the group of SL(2R) – type (for details see [7, 8]):

|  |      |
|--|------|
| $\begin{aligned} X' &= \alpha X + \beta Y \\ Y' &= \gamma X + \delta Y \\ \alpha\delta - \beta\gamma &= 1 \end{aligned}$ | (13) |
|--|------|

The basis of this Lie algebra is given by the infinitesimal generators:

|   |      |
|---|------|
| $X_1 = Y \frac{\partial}{\partial X}, \quad X_2 = \frac{1}{2} \left( X \frac{\partial}{\partial X} - Y \frac{\partial}{\partial Y} \right), \quad X_3 = -X \frac{\partial}{\partial Y}$ | (14) |
|---|------|



these generators satisfying the commutation relations:

$$[X_1, X_2] = X_1, \quad [X_2, X_3] = X_3, \quad [X_3, X_1] = -2X_2 \quad (15)$$

The solution of equations ((11), (12)) is written in the form:

$$[X(x)|Y(x)] = ze^{i(k_0x+\theta)} + \bar{z}e^{-i(k_0x+\theta)} \quad (16)$$

where  $z$  is a complex amplitude,  $\bar{z}$  is the complex conjugate of  $z$  and  $\theta$  is the specific phase. Thus, for a given polymer,  $z$ ,  $\bar{z}$  and  $\theta$  label each entity that have, as a general characteristic, the same  $k_0$ .

The equation (8) has a “hidden” symmetry in the form of a homographic group. Indeed, the ratio of two independent linear solutions of equation (8),  $\tau$ , is a solution of Schwartz’s differential equation [9]:

$$\begin{aligned} \{\tau, x\} &= \frac{d}{dx} \left( \frac{\ddot{\tau}}{\dot{\tau}} \right) - \frac{1}{2} \left( \frac{\ddot{\tau}}{\dot{\tau}} \right)^2 = 2k_0^2 \\ \dot{\tau} &= \frac{d\tau}{dx}, \quad \ddot{\tau} = \frac{d^2\tau}{dx^2} \end{aligned} \quad (17)$$

The left part of (17) is invariant with respect to the homographic transformation:

$$\tau \leftrightarrow \tau' = \frac{a_1\tau + b_1}{c_1\tau + d_1}, \quad (18)$$

with  $a_1, b_1, c_1$  and  $d_1$  real parameters. The relation (18) corresponding to all possible values of these parameters defines the group  $SL(2R)$ .

Thus, all the entities of the polymers having the same  $k_0$  are in biunivocal correspondence with the transformations of the group  $SL(2R)$ . This allows the construction of a “personal” parameter  $\tau$  for each entity of the polymer, separately. Indeed, as a “guide” it is chosen the general form of the solution of (17), which is written as:

$$\tau' = u + v \tan(k_0x + \theta) \quad (19)$$

So, through  $u, v$  and  $\theta$  it is possible to characterize any entity of the polymer.

In such a context, identifying the phase from (19) with the one from (16), the “personal” parameter of the entity becomes:

$$\tau' = \frac{z + \bar{z}\tau}{1 + \tau}, \quad z = u + iv, \quad \bar{z} = u - iv, \quad \tau \equiv e^{2i(k_0x+\theta)} \quad (20)$$

The fact that (20) is also a solution of (17) implies the following group, of  $SL(2R)$  – type (for details see [3, 4]):

$$\begin{aligned} z' &= \frac{a_1z + b_1}{c_1z + d_1} \\ k' &= \frac{c_1\bar{z} + d_1}{c_1z + d_1} k \end{aligned} \quad (21)$$

The infinitesimal generators of the group (21) are:

$$B_1 = \frac{\partial}{\partial z} + \frac{\partial}{\partial \bar{z}}, \quad B_2 = z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}}, \quad B_3 = z^2 \frac{\partial}{\partial z} + \bar{z}^2 \frac{\partial}{\partial \bar{z}} + (z - \bar{z})k \frac{\partial}{\partial k} \quad (22)$$

with commutation relations:

$$[B_1, B_2] = B_1, \quad [B_2, B_3] = B_3, \quad [B_3, B_1] = -2B_2 \quad (23)$$

The group (21) admits the differential 1- forms (absolutely invariant through the group) [3, 4, 10]:

$$\Omega_0 = -i \left( \frac{dk}{k} - \frac{dz + d\bar{z}}{z - \bar{z}} \right), \quad \Omega_1 = \frac{dz}{(z - \bar{z})k}, \quad \Omega_2 = -\frac{k d\bar{z}}{z - \bar{z}} \quad (24)$$

and the invariant metric:

$$\frac{ds^2}{f} = \Omega_0^2 - 4\Omega_1\Omega_2, \quad (25)$$

with  $f$  an arbitrary constant factor.

### 3. Results and discussions

An interesting case is the one induced by means of the parallel transport of direction in the Levy – Civita sense [3, 4, 10]. Then, in the space of variables  $(z, \bar{z}, k)$  the differential 1 – form  $\Omega_0$  is null:

$$\Omega_0 = 0, \quad (26)$$

while in the space of variables  $(u, v, \theta)$  is:

$$d\theta = -\frac{du}{v} \quad (27)$$

Since through (26) or (27) the invariant metric (25) is reduced to the Lobacevski plan metric in Poincaré representation, it results:

$$\frac{ds^2}{f} = \frac{dzd\bar{z}}{(z - \bar{z})^2} = \frac{du^2 + dv^2}{v^2} \quad (28)$$

In such a conjecture,  $\theta$  from (27) will define the angle of the parallel transport of direction in the Levy – Civita sense (for details [3, 4, 10]). Once the previous functionality is accepted (21), the infinitesimal generators of the group (18) become:

$$\bar{B}_1 = \frac{\partial}{\partial z} + \frac{\partial}{\partial \bar{z}}, \quad \bar{B}_2 = z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}}, \quad \bar{B}_3 = z^2 \frac{\partial}{\partial z} + \bar{z}^2 \frac{\partial}{\partial \bar{z}} \quad (29)$$

and satisfy the same commutation relations (23).

Now, consider another group of SL(2R) – type given by means of infinitesimal generators

$$\bar{H}_1 = \frac{\partial}{\partial h} + \frac{\partial}{\partial \bar{h}}, \quad \bar{H}_2 = h \frac{\partial}{\partial h} + \bar{h} \frac{\partial}{\partial \bar{h}}, \quad \bar{H}_3 = h^2 \frac{\partial}{\partial h} + \bar{h}^2 \frac{\partial}{\partial \bar{h}} \quad (30)$$

which satisfy the commutation relations:

$$[\bar{H}_1, \bar{H}_2] = \bar{H}_1, \quad [\bar{H}_2, \bar{H}_3] = \bar{H}_3, \quad [\bar{H}_3, \bar{H}_1] = -2\bar{H}_2 \quad (31)$$

Then, the Stoka system [11, 12] for operators (29) and (30) takes the form:

$$\begin{aligned}
 \frac{\partial F}{\partial h} + \frac{\partial F}{\partial \bar{h}} + \frac{\partial F}{\partial z} + \frac{\partial F}{\partial \bar{z}} &= 0 \\
 h \frac{\partial F}{\partial h} + \bar{h} \frac{\partial F}{\partial \bar{h}} + z \frac{\partial F}{\partial z} + \bar{z} \frac{\partial F}{\partial \bar{z}} &= 0 \\
 h^2 \frac{\partial F}{\partial h} + \bar{h}^2 \frac{\partial F}{\partial \bar{h}} + z^2 \frac{\partial F}{\partial z} + \bar{z}^2 \frac{\partial F}{\partial \bar{z}} &= 0
 \end{aligned}
 \tag{32}$$

It is important to notice that this system has the rank 3; as such, only one independent integral exists. This is the cross – ratio generated by means of the relation:

$$\frac{h - z}{h - \bar{z}} : \frac{\bar{h} - z}{\bar{h} - \bar{z}} \equiv \zeta^2,
 \tag{33}$$

where  $\zeta$  is real, and the square is taken in order to account for the fact that the cross – ratio (33) is always positive. Any joint invariant function,  $F$ , is here a regular function of this ratio. In such a context, if  $\zeta \equiv \tanh \phi$ , where  $\phi$  is arbitrary, then  $z$  is related to  $h$  through the linear relation:

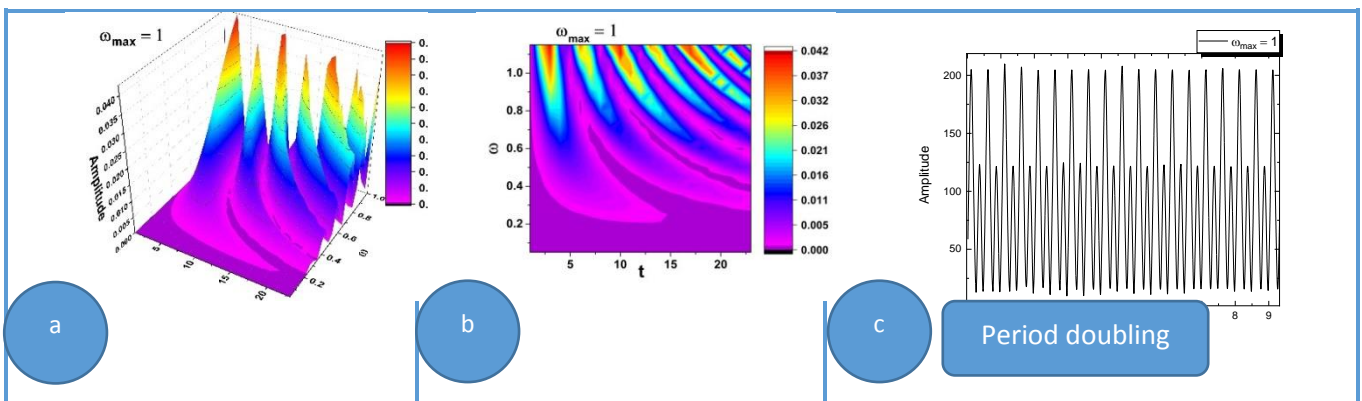
$$z = \bar{u} + \bar{v}h_0
 \tag{34}$$

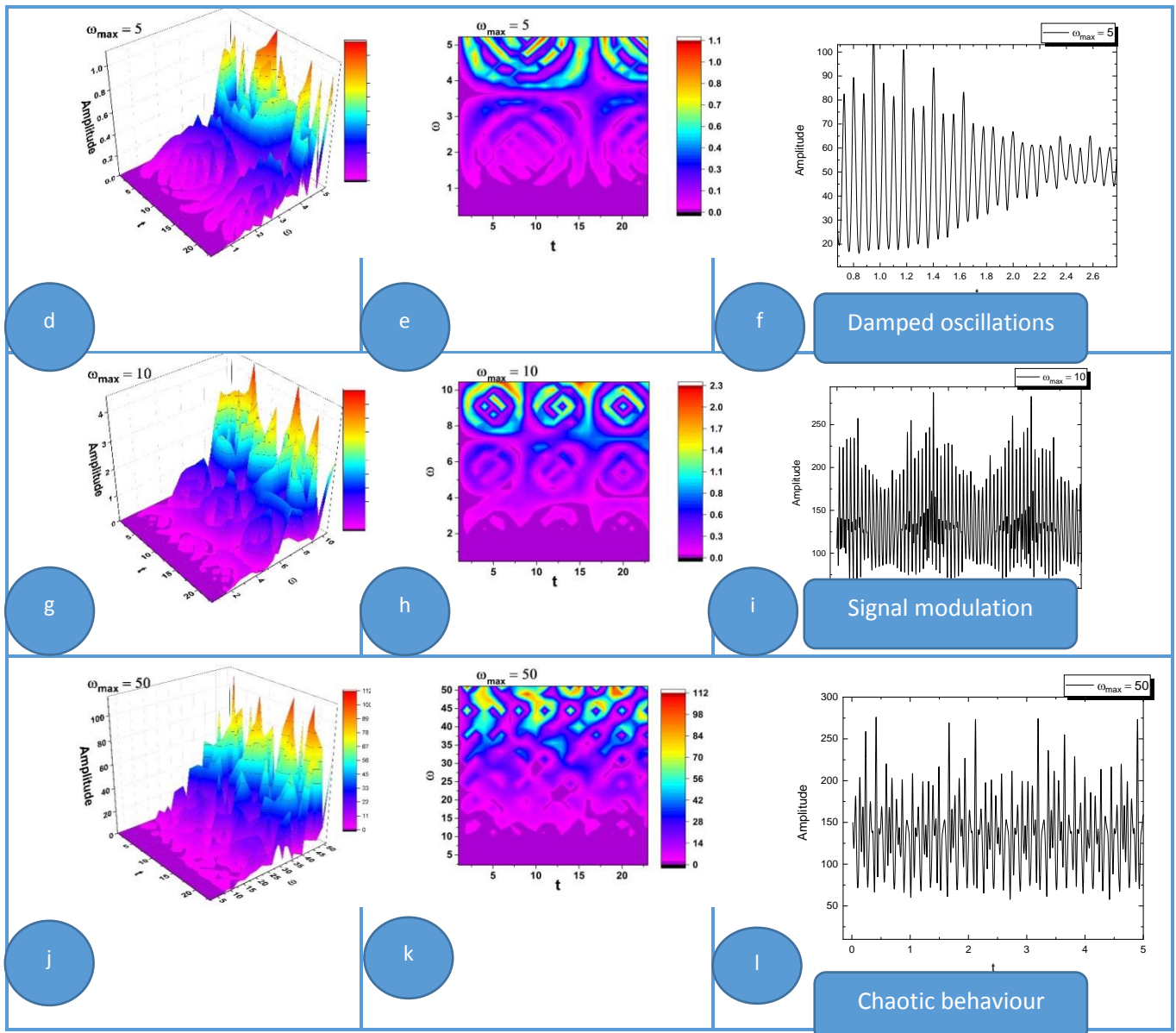
where

$$\begin{aligned}
 h &= \bar{u} + i\bar{v}, \quad i = \sqrt{-1} \\
 h_0 &= -i \frac{\cosh \phi - e^{-i\alpha} \sinh \phi}{\cosh \phi + e^{-i\alpha} \sinh \phi} \\
 \Delta \phi &= 0
 \end{aligned}
 \tag{35}$$

$\Delta$  is the Laplace operator and  $\alpha$  is real.

Therefore, synchronization of phase – amplitude type of each polymer entity (mathematically described through parallel transport of direction in Levi – Civita sense) implies joint invariant function of two simultaneous isomorphic groups of  $SL(2R)$  – type as solution of Stoka – type equation. Then, period doubling, damping oscillations, self – modulation and chaotic regimes emerge as natural behaviors in the polymer dynamics. (Figures 1 a – 1 for  $\alpha = \omega t$ ,  $\tanh \phi = 0.1$  and  $\text{Real} [(z - \bar{u}) / \bar{v}] \equiv \text{Amplitude}$  at various scale resolutions, given by means of the maximum value of  $\omega$ ). Let us note that synchronization types such as the ones mentioned above can be found in material structures in the form of self-structuring phenomena, from macroscale to nanoscale – for details [13-19].





**Figure 1.** Various types of synchronization of polymer entity (3D, contour plot and time series representation of the function signaling): period doubling (a, b, c), damped oscillation regime (d, e, f), signal modulation (g, h, i) and chaotic behavior (j, k, l))

#### 4. Conclusions

Various polymer dynamics in the fractal paradigm are proposed. Then:

i) The polymer structural units dynamics in the form of Schrodinger – type regimes imply various synchronization mechanisms of the polymer entities. In the most general case, the  $SL(2R)$  group works as a group of “synchronism” among the various entities of the polymer, process to which the amplitudes and phases of each of them obviously participate, in the sense that they are also connected. More precisely, by means of  $SL(2R)$  group, the phase is only moved with a quantity depending on the amplitude of the polymer structural unit at the transition among various entities of the polymer. More than that, the amplitude of the polymer structural unit is also affected from a homographic perspective. The usual “synchronization” manifested through the delay of the amplitudes and phases of the polymer entities must represent here only a fully particular case.

ii) In the case of synchronization, which implies reciprocal conditions of phase – amplitude type of each polymer structural unit (mathematically described through parallel transport of direction in Levi – Civita sense), joint invariant function of two simultaneous isomorphic groups of  $SL(2R)$  – type



as solution of Stoka – type equation, are revealed. Then, period doubling, damping oscillations, self – modulation and chaotic regimes emerge as natural behaviors in the polymer structural units dynamics.

This model may be extended to use to other classes of materials, such as biomaterials, biocomposites and other advanced materials.

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