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BIFURCATIONS AND CHAOS OF DNA SOLITONIC DYNAMICS

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ABSTRACT

We investigated the nonlinear DNA torsional equations proposed by Yakushevich [1] in the presence of damping and external torques. Analytical expressions for some solutions are obtained in the case of the isolated chain. Special attention is paid to the stability of the solutions and the range of soliton interaction in the general case. The bifurcation analysis is performed and prediction of chaos is obtained for some set of parameters. Some biological implications are suggested.

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1 Introduction

Some nonlinear dynamical models have been proposed [1-3] for DNA in order to explain the origin and dynamics of open states in this molecule [4-6] which are somehow related to the transcription or replication processes. The interaction between the solitons (or open states) are variable for different proposed models and in most cases are short range. In this paper we study a particular model [1] which describes the torsional dynamics of the double DNA helix and we obtain the general behaviour of the solutions and the range of the interaction between the solitons, which turned out to be long-range. We also investigated the influence of damping, external fields and torques in the dynamics of the solitons.

In the quoted article [1], Yakushevich proposed the following equations for the torsional dynamics of DNA:

$$I_1 \varphi_{1_{tt}} = K_1 a^2 \varphi_{1_{zz}} - k\frac{\Lambda I}{I}[(2R^2 + RI_0)\sin\varphi_1 - R^2(\varphi_1 + \varphi_2)] \quad (1.a)$$

$$I_2 \varphi_{2_{tt}} = K_2 a^2 \varphi_{2_{zz}} - k\frac{\Lambda I}{I}[(2R^2 + RI_0)\sin\varphi_2 - R^2(\varphi_1 + \varphi_2)] \quad (1.b)$$

where:

$$\frac{\Delta l}{l} = 1 - l_0\left[(2R + l_0 - R\cos\varphi_1 - R\cos\varphi_2)^2 + (R\sin\varphi_1 - R\sin\varphi_2)^2\right]^{-\frac{1}{2}}$$

In these equations, φ_i is the torsional angle, I_i is the moment of inertia, K_i is the rigidity of the longitudinal springs of the i-th chain, k the rigidity of the transversal spring connecting both chains, R the radius of the chains, l_0 is the minimum separation between the chains and a is the characteristic length of the base pair in the double helix. In Reference 1 these are simplified by assuming that l_0 0, which leads to:

$$I_1\varphi_{1tt} - K_1a^2\varphi_{1zz} + kR^2|2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)| = 0 \qquad (2.a)$$

$$I_2\varphi_{2tt} - K_2a^2\varphi_{2zz} + kR^2|2\sin\varphi_2 - \sin(\varphi_1 + \varphi_2)| = 0 \qquad (2.b)$$

For these equations different types of solutions are proposed in order to simplify even more the set of equations. The following cases are considered as solutions of equations (2):

case a) $\varphi_1 = 0$, $\varphi_2 \neq 0$, for which the equations (2) are reduced to:

$$I\varphi_{tt} - Ka^2\varphi_{zz} + kR^2\sin\varphi = 0 \qquad (3)$$

This result is not quite correct since by putting $\varphi_1 = 0$ in equation (2.a) then $\sin\varphi_2 = 0$, which leads necessarily to the solution $\varphi_2 = n\pi$ $const.$, and does not correspond to a solitonic solution of equation (3).

On the other hand, cases b) $\varphi_1 = \varphi_2$ and c) $\varphi_1 = -\varphi_2$ lead to the equations:

$$I\varphi_{tt} - Ka^2\varphi_{zz} + 2kR^2\sin\varphi - kR^2\sin 2\varphi = 0 \qquad (4)$$

and

$$I\varphi_{tt} - Ka^2\varphi_{zz} + 2kR^2\sin\varphi = 0 \qquad (5)$$

respectively. These equations are only valid for symmetric chains, i.e., $I_1 = I_2 = I$ and $K_1 = K_2 = K$.

II.- Qualitative Analysis.

Let us make the analysis of equation (2) in a more general way. As it is of common usage, let us introduce the travelling wave variable $\zeta = z - vt$, where v is a constant, to obtain the following system of equations:

$$W_1\varphi_1'' - kR^2[2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)] = 0 \qquad (6.a)$$

$$W_2\varphi_2'' - kR^2[2\sin\varphi_2 - \sin(\varphi_1 + \varphi_2)] = 0 \qquad (6.b)$$

where $W_i = K_i a^2 - I_i v^2$ and the prime corresponds to the derivative with respect to ζ. The system of equations (6) can be written as:

$$W_1\varphi_1'' = -\frac{\partial V(\varphi_1,\varphi_2)}{\partial\varphi_1} \qquad (7.a)$$

$$W_2\varphi_2'' = -\frac{\partial V(\varphi_1,\varphi_2)}{\partial\varphi_2} \qquad (7.b)$$

where

$$V(\varphi_1,\varphi_2) = kR[2(\cos\varphi_1 + \cos\varphi_2) - \cos(\varphi_1 + \varphi_2)] \qquad (8)$$

$V(\varphi_1, \varphi_2)$ has local maxima at the point $\varphi_1 = 2n\pi$, $\varphi_2 = 2m\pi$, with $n = 0, \pm 1, \pm 2, \ldots$, and $m = 0, \pm 1, \pm 2, \ldots$. The points $\varphi_1 = (2n-1)\pi$, $\varphi_2 = (2m-1)\pi$ correspond to local minima, while the points $\varphi_1 = (2n-1)\pi$, $\varphi_2 = 2m\pi$; $\varphi_1 = 2n\pi$, $\varphi_2 = (2m-1)\pi$ are saddle points. These points are shown in Figure 1. In the figure are shown the phase plane trajectories joining critical points which correspond to solitons.

The local maxima have the same height so for every two contiguos local maxima there are solutions of the kink type [7,8]. For example, there are solutions with the following properties:

$$\lim_{\varsigma \to -\infty} \varphi_1 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_1 = +2\pi$$

$$\lim_{\varsigma \to -\infty} \varphi_2 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_2 = 0 \qquad (9.1)$$

$$\lim_{\varsigma \to -\infty} \varphi_1 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_1 = 0$$

$$\lim_{\varsigma \to -\infty} \varphi_2 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_2 = +2\pi \qquad (9.2)$$

$$\lim_{\varsigma \to -\infty} \varphi_1 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_1 = 0$$

$$\lim_{\varsigma \to -\infty} \varphi_2 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_2 = -2\pi \qquad (9.3)$$

$$\lim_{\varsigma \to -\infty} \varphi_1 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_1 = +2\pi$$

$$\lim_{\varsigma \to -\infty} \varphi_2 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_2 = +2\pi \qquad (10.1)$$

$$\lim_{\varsigma \to -\infty} \varphi_1 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_1 = +2\pi$$

$$\lim_{\varsigma \to -\infty} \varphi_2 = 0, \quad \lim_{\varsigma \to +\infty} \varphi_2 = -2\pi \qquad (10.2)$$

and their antikink solitons respectively. See Figures (2 - 8). Note that the points *(0,0)* and *(2π,2π)* are linked by a single trajectory, while the points *(0,0)* and *(2π,-2π)* are connected by three different trajectories. For further reference we will call those three trajectories as (10.2.1), (10.2.2) and (10.2.3) after Figure 1.

Among these solutions those of the type (9) are strictly stable. The solutions given by (10) may decompose into two solitons of the type (9), together with small amplitude travelling waves. We must also notice that the connection of the points *(0,0)* and *(0,2π)* can not be done through the straight line $\varphi_1 = 0$, which is due to the fact that $\varphi_1 = 0$, $\varphi_2 \neq 0$ is not a solitonic solution of equation (3).

There are different critical velocities for $K_1 \neq K_2$, given by the general expression:

$$c_i = \frac{K_i a^2}{I_i} \qquad (11)$$

and the velocity of this kind of soliton will be restricted to $0 < v^2 < c_m^2$, with c_m the minimum critical velocity.

III.- Some Analytical Solutions.

The cases b) and c), represented by equations (4) and (5) correspond to solutions of the type given by (10). For the last case (case c)), we have the following exact solutions:

$$\varphi_1 = -\varphi_2 = 4\arctan\left[\exp\left[\frac{z - z_0 - vt}{\Lambda_0 \gamma}\right]\right] \qquad (12)$$

where $\gamma = \sqrt{1 - \frac{v^2}{c^2}}$, $\Lambda_0 = \frac{Ka^2}{kR^2}$, $c^2 = \frac{Ka^2}{I}$, z_0 is the initial position of the soliton and v its traslational velocity. The rest energy, i.e., the energy necessary to produce a static open state, is the following:

$$H_{0\,(\varphi_1 - \varphi_2)} = 16\sqrt{2Kk}\,aR \qquad (13)$$

and the total energy for a travelling soliton is related to the rest energy through the Lorentz factor, $H = \frac{H_0}{\gamma}$.

For case b), i.e., $\varphi_1 = \varphi_2$, we have:

$$\varphi_1 = \varphi_2 = 2\arctan\left[\sqrt{2}\left[\frac{z - z_0 - vt}{\Lambda_0 \gamma}\right]\right] + \pi \qquad (14)$$

For this case, the rest energy is given by:

$$H_{0\,(\varphi_1 - \varphi_2)} = 4\pi\sqrt{2Kk}\,aR \qquad (15)$$

Note that in equations (14) there are no exponentials in the argument of the arctan function. The solution of the type described by equations (12) will be called asymmetric, while the solutions (14) will be called symmetric. Both types of solutions are shown in Figures (5-6). We have constructed an approximated analytical solution function for type (9.1) solutions (see Figures 2 through 4).

$$\varphi_1 = 2\arctan\left[\frac{N\zeta}{\Lambda_0}\right] + \pi \qquad (16)$$

$$\varphi_2 = N_1 \arctan\left[\frac{\sin\left[2\arctan\left[\frac{N_2\zeta}{\Lambda_0}\right]+\pi\right]}{2-\cos\left[2\arctan\left[\frac{N_2\zeta}{\Lambda_0}\right]+\pi\right]}\right] \qquad (17)$$

where $N = 1.2586$, $N_1 = 0.75945$ and $N_2 = 1.1222$.

We also constructed approximated analytical solutions for type (10.2.2) and type (10.2.3) solutions:

$$\varphi_1 = 2\arctan[N_{11}[\zeta - \zeta_{11}]] + \pi - N_1\arctan\left[\frac{\sin[2\arctan(\zeta+\zeta_{12})+\pi]}{2-\cos[2\arctan(\zeta+\zeta_{12})+\pi]}\right] \qquad (18)$$

$$\varphi_2 = -2\arctan[N_{21}[\zeta + \zeta_{21}]] - \pi + N_2\arctan\left[\frac{\sin[2\arctan(\zeta-\zeta_{22})+\pi]}{2-\cos[2\arctan(\zeta-\zeta_{22})+\pi]}\right] \qquad (19)$$

where $N_{11} = N_{21} = 1.2250$, $\zeta_{11} = \zeta_{21} = 2.4836$, $N_1 = N_2 = 0.86111$, $\zeta_{12} = \zeta_{22} = 1.2228$ for solution (10.2.3). These solutions are shown in Figures 7 - 8.

For the type of solution described in equation (9), the rest energy can be written approximately as:

$$H_0 = 8\sqrt{2Kk}\,aR \qquad (20)$$

By comparing the energies for the unstable states (asymmetric and symmetric), given by equations (13) and (15) respectively, with the energy of the stable soliton, equation (20), it is possible in principle to calculate the energy radiated through the generation of small amplitude travelling waves.

The system described by equations (7) can be written as an autonomous dynamical system:

$$\varphi_1' = \theta_1$$

$$\theta_1' = \frac{kR^2}{W_1}[2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)]$$

(21)

$$\varphi_2' = \theta_2$$

$$\theta_2' = \frac{kR^2}{W_2}[2\sin\varphi_2 - \sin(\varphi_1 + \varphi_2)]$$

The eigenvalues of the Jacobi matrix at the critical points of system (21) $\varphi_1 = 2\,n\,\pi$, $\varphi_2 = 2\,m\,\pi$, are the following:

$$(\lambda_{1,2})^2 = 0 \qquad (22)$$

$$(\lambda_{3,4})^2 = \frac{kR^2}{W_1} + \frac{kR^2}{W_2} \qquad (23)$$

The eigenvalues equal to zero, (equation (22)), reflect that there are some degeneracy at the critical points and also there is some anysotropy at these points reflected by the fact that the behavior of the solitons produced along the line $\varphi_1 = \varphi_2$ is different from that along $\varphi_1 = -\varphi_2$. This difference in behavior can be seen for the solutions given by the equations (12) and (14). For the former there is a fast exponential behavior at the tails of the soliton when $\zeta \to \pm\infty$, while for the second type, the behavior is somewhat slower. Recalling that:

$$\varphi' = [2\arctan(B\zeta) + \pi]' = \frac{2B}{1+(B\zeta)^2} \qquad (24)$$

where $B = \sqrt{\frac{2kR^2}{W}}$, i.e., it means that $\varphi' \sim \frac{1}{\zeta^2}$ and $\varphi \sim \frac{1}{\zeta}$ when $\zeta \to \pm\infty$. This result is important for the type of interaction between solitons and will be discussed later in this work.

IV.- Stability Analysis.

Now we will study the stability of the solutions. Let us assume that $I_1 = I_2 = I$, $K_1 = K_2 = K$ to simplify calculations. Then:

$$\frac{1}{c^2}\varphi_{1tt} - \varphi_{1zz} + \frac{1}{\Lambda_0^2}[2\sin\varphi_1 - \sin(\varphi_1 + \varphi_2)] = 0 \tag{25.a}$$

$$\frac{1}{c^2}\varphi_{2tt} - \varphi_{2zz} + \frac{1}{\Lambda_0^2}[2\sin\varphi_2 - \sin(\varphi_1 + \varphi_2)] = 0 \tag{25.b}$$

Let $\varphi_{1k}(z)$ and $\varphi_{2k}(z)$ be solitonic solutions of system (25). We will perturbate slightly these solitonic solutions and will determine if these perturbations remain small with time. Making $\varphi_1 = \varphi_{1k} + \psi_1$ and $\varphi_2 = \varphi_{2k} + \psi_2$, we obtain for ψ_1 and ψ_2 the following equations:

$$\frac{1}{c^2}\psi_{1tt} - \psi_{1zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_{1k})\psi_1 - \cos(\varphi_{1k} + \varphi_{2k})(\psi_1 + \psi_2)] = 0 \tag{26.a}$$

$$\frac{1}{c^2}\psi_{2tt} - \psi_{2zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_{2k})\psi_2 - \cos(\varphi_{1k} + \varphi_{2k})(\psi_1 + \psi_2)] = 0 \tag{26.b}$$

By putting $\psi_1 = f_1(z)\, e^{\lambda t}$ and $\psi_2 = f_2(z)\, e^{\lambda t}$, we state an eigenfunction and eigenvalue problem:

$$-f_{1zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_{1k})f_1 - \cos(\varphi_{1k} + \varphi_{2k})(f_1 + f_2)] = \Gamma f_1 \tag{27.a}$$

$$-f_{2zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_{2k})f_2 - \cos(\varphi_{1k} + \varphi_{2k})(f_1 + f_2)] = \Gamma f_2 \tag{27.b}$$

where $\Gamma = -\frac{\lambda^2}{c^2}$.

If we can demonstrate that the spectral problem (27) does not posses solutions corresponding to values of λ with positive real part then the soliton under study is stable.

We have found that the type (9) solitons are stable while the type (10) are composite structures of the former. In some cases these unions are totally unstable and in others it is necessary some perturbation to decompose it in a pair of solitons.

For example, the case $\varphi_{1k} = -\varphi_{2k} = \varphi_k = 4\arctan\left[\exp\left[\frac{\sqrt{2}\,z}{\Lambda_0^2}\right]\right]$ (solitons of type (10.2.1)). In this case

$$-f_{1zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_k)f_1 - f_1 - f_2] = -\frac{\lambda^2}{c^2}f_1 \qquad (28.a)$$

$$-f_{2zz} + \frac{1}{\Lambda_0^2}[2\cos(\varphi_k)f_2 - f_1 - f_2] = -\frac{\lambda^2}{c^2}f_2 \qquad (28.b)$$

There are two eigenvalues corresponding to a discrete spectrum. The solution corresponding to the eigenvalue $\lambda_1 = 0$ is:

$$f_{11} = -f_{21} = \frac{d\varphi_k}{dz} = \frac{4\frac{\sqrt{2}}{\Lambda_0}}{\cosh\left[\frac{\sqrt{2}\,z}{\Lambda_0}\right]} \qquad (29)$$

For the positive eigenvalue $\lambda_2 = \sqrt{2}\frac{c}{\Lambda_0}$, we have the solution:

$$f_{12} = -f_{22} = -\frac{4\frac{\sqrt{2}}{\Lambda_0}}{\cosh\left[\frac{\sqrt{2}\,z}{\Lambda_0}\right]} \qquad (30)$$

The rest of the eigenvalues are imaginary (continuous spectrum). For type (9) solutions, i.e., $\varphi_{1k} \approx 4\arctan\left[\exp\left[\frac{z}{\Lambda_0}\right]\right]$, $\varphi_{2k} \approx 0$, system (26) is topologically equivalent to:

$$\frac{1}{c^2}\psi_{1tt} - \psi_{1zz} + \frac{1}{\Lambda_0}|\cos(\varphi_{1k})\psi_1| = 0 \qquad (31.a)$$

$$\frac{1}{c^2}\psi_{2tt} - \psi_{2zz} + \frac{2}{\Lambda_0}\psi_2 = 0 \qquad (31.b)$$

which contains the classical sine-Gordon solitons with a single eigenvalue corresponding to the discrete spectrum ($\lambda = 0$) and a continuous spectrum. These solitons are stable.

Solitons of type (10.1) are unstable. Even while solitons of type (10.2.2) and (10.2.3) are stable under small perturbations, they can decompose into one type (9.1) and one type (9.3) solitons under strong perturbations.

V.- The Exact Model.

Let us now study the general system (1) with $l_0 \neq 0$. In this case the solitons are solutions of the system:

$$W_1\varphi_1'' = -\frac{\partial V(\varphi_1,\varphi_2)}{\partial \varphi_1} \qquad (32.a)$$

$$W_2\varphi_2'' = -\frac{\partial V(\varphi_1,\varphi_2)}{\partial \varphi_2} \qquad (32.b)$$

where:

$$V(\varphi_1,\varphi_2) = -\frac{1}{2}kR^2\left[\sqrt{\left(2+\frac{l_0}{R} - \cos\varphi_1 - \cos\varphi_2\right)^2 + (\sin\varphi_1 - \sin\varphi_2)^2} - \frac{l_0}{R}\right]^2 \qquad (33)$$

and the first integral is:

$$\frac{1}{2}W_1\varphi_1'^2 + \frac{1}{2}W_2\varphi_2'^2 + V(\varphi_1,\varphi_2) = const. \qquad (34)$$

From a qualitative point of view, the potential energy $V(\varphi_1, \varphi_2)$ for the exact system is not different from the one described in Figure 1, i.e., the solitonic solutions connect the same critical points. However, there is a quantitative difference between both situations.

The eigenvalues of the Jacobi matrix at the points $\varphi_1 = 2n\pi$, $\varphi_2 = 2m\pi$ for the system (24) are all equal to zero. This result means that there is no optical branch in the vibrational spectrum for the general system (24), in contradiction to what is claimed in Reference 1.

In the neighborhood of the points $\varphi_1 = 2n\pi$ and $\varphi_2 = 2m\pi$, the function $V(\varphi_1, \varphi_2)$ has the following behavior:

$$V(\varphi_1, \varphi_2) = -\frac{1}{2}kR^2\left[\frac{1}{4}\left(1+\frac{1}{\varepsilon}\right)^2\left(\varphi_1^4+\varphi_2^4\right) - \frac{1}{\varepsilon}\left(1+\frac{1}{\varepsilon}\right)\left(\varphi_1^3\varphi_2+\varphi_1\varphi_2^3\right)+\left(\frac{3}{2\varepsilon^2}+\frac{1}{\varepsilon}+\frac{1}{2}\right)\varphi_1^2\varphi_2^2\right] \qquad (35)$$

where $\varepsilon = \frac{l_0}{R}$.

These points are completely degenerate and in its neighborhood, equations (34) do not show linear terms. According to (35), the terms different from zero in the expansion of $V(\varphi_1, \varphi_2)$ are of fourth order. This dependence is of particular importance in the properties of the solitons, its dynamics and interactions [9]. First, as it was shown in equations (24), the asymptotical behavior of the solitons at the critical point is as $\varphi \sim \frac{1}{\zeta}$, which means that the interaction between the solitons is long range. In Reference 9, it was demonstrated that if the local behavior for the potential at the critical points is as φ^{2n}, $n > 1$ then the interaction force between the solitons decreases with the distance r as:

$$F \sim r^{\frac{2n}{1-n}} \qquad (36)$$

The interaction force between the solitons for the system (1) with $l_0 \neq 0$ decreases with the distance as:

$$F \sim r^{-4} \qquad (37)$$

Some exact solutions when $l_0 \neq 0$ are obtained for different cases, assuming that $W_1 = W_2$ and $c_1 = c_2 = c$: a) $\varphi_1 = -\varphi_2 = \varphi$,

$$\int_0^{\varphi} \frac{d\varphi'}{\sqrt{\varepsilon^2+4(2+\varepsilon)(1-\cos\varphi')}-\varepsilon} = \frac{z-z_0-vt}{\sqrt{2}\,\Lambda_0\gamma} \quad ; \tag{38}$$

and b) $\varphi_1 = \varphi_2 = \varphi$:

$$\varphi = 2\arctan\left[\frac{\sqrt{2}}{\Lambda_0}\frac{z-z_0-vt}{\gamma}\right] + \pi \tag{39}$$

When $I_0 \neq 0$, the behavior of all solitonic solutions is asymptotically slower than exponential.

VI.- The Perturbed Model.

So far we have studied the undriven Yakushevich equation. Of unquestionable interest is the influence of damping and external torsions on the solutions.

$$I_1\varphi_{1tt} + \gamma_1\varphi_{1t} - K_1a^2\varphi_{1zz} - k\frac{\Delta l}{l}\left[(2R^2+Rl_0)\sin\varphi_1 - R^2\sin(\varphi_1+\varphi_2)\right] = H_1$$

(40.a)

$$I_2\varphi_{2tt} + \gamma_2\varphi_{2t} - K_2a^2\varphi_{2zz} - k\frac{\Delta l}{l}\left[(2R^2+Rl_0)\sin\varphi_2 - R^2\sin(\varphi_1+\varphi_2)\right] = H_2$$

(40.b)

The damping forces $\gamma_1\varphi_{1t}$ and $\gamma_2\varphi_{2t}$ tend to slow down the solitons.

Before analyzing the global action of the torsional forces H_1 and H_2, we will study the local bifurcations they produce.

As shown before, the critical points $(2n\pi, 2m\pi)$ are degenerated (their eigenvalues are equal to zero). Under the effect of the torsional forces the system bifurcates and the resulting critical points are Morse type. So the original model is structurally unstable under perturbations in the form of torsional forces like in equations (40).

To simplify the analysis we will use the approximation $l_0 = 0$ and we will concentrate on the point *(0,0)* (see Figure 9 for reference and recall that the system is invariant under the transformation $\varphi^* = \varphi_i \pm 2\pi$).

In the cross hatched area the system has only one critical point close to zero. This point corresponds to the minimum of potential $U(\varphi_1, \varphi_2) = -V(\varphi_1, \varphi_2)$ and therefore is stable.

In the point hatched area the system has three critical points close to zero, two stable and one unstable. Moving in that area and varying the values of h_1 and h_2 with $h_i = \frac{H_i}{\lambda R^2}$ in such a way as to pass to the cross hatched area then a bifurcation with the union of two of those three points (the unstable and one of the stable) so both of them dissapear. If from the point hatched area we cross to the solid filled one then one of the stable points merges with an unstable point belonging to a zone not related to the point *(0,0)* (a saddle point of $U(\varphi_1, \varphi_2)$) and in a vicinity of the zero still remain two points: one stable and one unstable.

If we pass from the hatched areas to those which aren't, then we will not have critical points close to zero, i.e., the sole remaining point merges with a saddle point or a maximum of $U(\varphi_1, \varphi_2)$, while if we are in the solid filled area the remaining points annihilate between themselves. In that case the system has no solitonic solutions, recalling that the solitons are formed by connections between the maxima of $V(\varphi_1, \varphi_2)$ (minima of $U(\varphi_1, \varphi_2)$).

If a soliton connects to points, for example $(\varphi_{11}, \varphi_{21})$ and $(\varphi_{12}, \varphi_{22})$, then the value of $\Delta = U(\varphi_{11}, \varphi_{21}) - U(\varphi_{12}, \varphi_{22})$ plays an important part in its dynamics.

For the kinks, $\Delta > 0$ acts as an external force on the kink pushing it in the positive sense of the z axis and inversely if $\Delta < 0$. The effect on the antikink is exactly the opposite. If $\Delta = 0$, the soliton can exist at rest.

When besides the condition $\Delta \neq 0$, we have damping then the soliton acquires a stable velocity proportional to Δ and inversely proportional to the damping coefficients γ_i. In our system:

$$\Delta = -\left[H_1(\varphi_{12} - \varphi_{22}) + H_2(\varphi_{11} - \varphi_{21})\right] \qquad (41)$$

For example, if $h_1 > 0$ and $h_2 > 0$, the type (9.1) and (9.2) solitons are accelerated in the negative sense of the z axis while the antisolitons would move in the opposite sense. But type (9.3) solitons will behave in the opposite way. When we refer to type (9.1) or other solitons we are addressing solitons joining points in the vicinity of those assigned by the formulae referenced because when $h_1 \neq 0$, $h_2 \neq 0$, the critical points are not in $(2n\pi, 2m\pi)$.

Some interesting situations occur when $|h_1| = |h_2|$. For $h_1 = h_2 = h > 0$, type (10.2.2) and (10.2.3) solitons can exist at rest as $\Delta = 0$. If $h_1 = -h_2 = h > 0$, then type (10.1) can exist at rest. In that case, an extremely interesting soliton can also exist at rest, which connects two critical points corresponding to minima of $U(\varphi_1, \varphi_2)$ (or maxima of $V(\varphi_1, \varphi_2)$), since we are moving in the point hatched area in Figure 9 and for those points $\Delta = 0$. We have called this soliton, a baby-soliton, because its amplitude is extremely small and it is shown in Figure 10.

VII.- General Dynamics.

We will introduce some definitions to classify and explain all the solitonic interactions that occur in these systems.

Let us define topological charge q_t and chain charge q_c as:

$$q_t = \frac{(\varphi_1(\infty) - \varphi_1(-\infty)) + (\varphi_2(\infty) - \varphi_2(-\infty))}{2\pi} \qquad (42)$$

$$q_c = \frac{|\varphi_1(\infty) - \varphi_1(-\infty)| - |\varphi_2(\infty) - \varphi_2(-\infty)|}{2\pi} \qquad (43)$$

If two solitons have chain charge of equal sign, then the fundamental interaction among themselves is of topological type. In that case two solitons with topological charge of equal sign repel each other while two possesing topological charges of different sign attract each other. Then it is not odd that breathers are formed by the interaction of a kink and antikink in type (9) solitons if they both have equal chain charge.

If two solitons have different sign of the chain charge then, on top of the topological interaction there is a repulsive force produced by the chain interaction. This interaction force is zero when the distance between the center of mass of the solitons is zero (see Figure 11). It reaches its maximum for a distance different from zero and then decreases rapidly with the distance. The repulsive force produced by the chain interaction is of smaller range than the topological interaction force, but the chain repulsive force is stronger when the solitons have topological charge of different sign. Of course the effective interaction force is repulsive only for short distances. At greater distances always prevails the attractive topological force.

The presence of external forces leading to $\Delta \neq 0$ influence the solitons through the topological charge. If $\Delta > 0$, the solitons with positive topological charge are accelerated in the positive sense of the z axis while those with negative topological charge are accelerated in the negative sense. If $\Delta < 0$, the opposite happens. This result is more general than the one for kinks and antikinks because is valid also for compounded structures with topological charge different from those of kink and antikink and even zero.

These "laws" explain all the phenomena detected in the system (40), whether as theoretical results or as found by numerical experiments.

The unstability of type (10.1) solitons is due to their being composed of a type (9.1) and a type (9.2) kink. In that case the slightest perturbation displacing their respective centers of mass allows the repulsive force to star sparating them.

The same happens with type (10.2.1) solitons which are composed with a type (9.1) and a (9.3). As these solitons have topological charge of unequal sign, then for big distances the topological attraction prevails.

A compromise between those two opposing forces produce type (10.2.2) and (10.2.3) solitons. In these composite structures the centers of mass of both the (9.1) and (9.3) solitons are displaced.

In principle it is posible to define solitonic reactions. For example:

$$(10.1) \rightarrow (9.1)+(9.2)+\Delta E \qquad \text{(I)}$$

$$(10.2.1) \rightarrow (9.1)+(9.3)+\Delta E \qquad \text{(II)}$$

$$(10.2.1) \rightarrow (10.2.2) \quad +\Delta E \qquad \text{(III)}$$

In these reactions the energy, the topological charge and the linear momentum are conserved. the energy liberated can be determined calculating the energy difference between the initial and final states. Note that in equations (13), (15) and (20) the rest energy of the composite states is higher than the rest energy of type (9) solitons.

It is important to point out that the reaction (III) could only occur if there is damping, because the rest energy of state (10.2.1) is much bigger than that of state (10.2.2) and the kinetic energy acquired by the (9.1) and (9.3) solitons by the reaction (II), since linear momentum is conserved, is very high so the attracting force is not able to stop the accelerated separation of the solitons. Only the damping is able to slow down enough the emerging type (9) solitons and to stabilize in a type (10.2.2).

In a damped system the stable states are spatio-temporal attractors and any initial condition close to those states leads inevitably to them. We must point out that our analysis shows that the equations of Yakushevich are non integrable because the interaction between the solitons is unelastic.

Type (10.1) solitons can be stabilized using torsional forces of equal modulo but different sign $h_1 = -h_2 = h$. To achieve this we must use as initial condition a type (9.1) and (9.2) solitons with displaced centers of mass. It produces an equilibrium between the repulsive force among them and the external torsional forces, one acting in one direction on one soliton and the other acting on the other soliton in the opposite direction.

A similar state can be achieved by coupling type (9.1) and (9.3) solitons but now using $h_1 = h_2$ (see Figures 12 and 13). The baby-soliton mentioned above is due to the same cause. Note that the last two composite states have zero topological charge. With a fixed relative position of the centers of mass, they have traslational freedom.

It is interesting to notice that when type (10.1) solitons are perturbed by external torsional forces such as $h_1 > 0$, $h_2 = 0$, then the solitons (9.1) and (9.2) composing it move as a whole, because when over the one on the right acts an external force in the negative sense it pushes (by the repulsive interaction) the one on the left.

All this phenomena has been corroborated with the aid of numerical experiments.

When $\Delta \neq 0$, for two critical points of the system bell-solitons can form which are no more than linked kink-antikink states [7,9].

There is a critical distance when the atractive forces between kink and antikink are equilibrated with the external force separating them. The result is unstable. Beginning with an initial condition where a kink and an antikink are at a distance which is lower than the critical one, the solitons tend to get closer. If the initial distance between the solitons is above the critical value then the external force do separate them.

VIII.- Chaos.

Let us return to the equations of the unperturbed exact model. In the vicinity of the equilibrium points $(\varphi_1 = 2n\pi, \varphi_2 = 2m\pi)$ the equations (1) appear as:

$$I_1\varphi_{1tt} - K_1a^2\varphi_{1zz} = \frac{1}{2}kR^2\left[\left(1-\frac{1}{\varepsilon}\right)^2\varphi_1^3 - \frac{1}{\varepsilon}\left(1+\frac{1}{\varepsilon}\right)\left(3\varphi_1^2\varphi_2+\varphi_2^3\right)+2\left(\frac{3}{2\varepsilon^2}+\frac{1}{\varepsilon}+\frac{1}{2}\right)\varphi_1\varphi_2^2\right]$$

(44.a)

$$I_2\varphi_{2tt} - K_2a^2\varphi_{2zz} = \frac{1}{2}kR^2\left[\left(1-\frac{1}{\varepsilon}\right)^2\varphi_2^3 - \frac{1}{\varepsilon}\left(1+\frac{1}{\varepsilon}\right)\left(3\varphi_2^2\varphi_1+\varphi_1^3\right)+2\left(\frac{3}{2\varepsilon^2}+\frac{1}{\varepsilon}+\frac{1}{2}\right)\varphi_2\varphi_1^2\right]$$

(44.b)

Note that the terms in the right hand side of the equations are of 3rd order.

If these equations are perturbed by periodic forces and dissipation, the dynamical behavior will be in some sense similar to that of the cubic Duffing equation [10]:

$$\frac{d^2x}{dt^2}+\gamma\frac{dx}{dt}+Ax^3 = F_0\cos(\omega t) \qquad (45)$$

which is well known to have a chaotic attractor. This result means that in addition to the expected chaotic behavior in the periodically perturbed DNA system (1) due to the nonintegrability of these equations and the homoclinic loops that they contain, we can predict chaotic oscillations around the equilibrium points. Due to this phenomenon, the tails of the solitons will perform chaotic oscillations.

As we saw in Section VI, when the external torsional forces are of equal modulo but different sign, the system bifurcates and the equilibrium points $\varphi_1 = 2n\pi$, $\varphi_2 = 2m\pi$ degenerate in three points, two stable and one unstable. If we now drive the system with a periodical force, it will perform oscillations similar to those described by Duffing's equations, but now with several critical points [11].

$$\frac{d^2x}{dt^2}+\gamma\frac{dx}{dt} - x+Ax^3 = F_0\cos(\omega t) \qquad (46)$$

For several values of the parameters the equation (46) has a chaotic attractor. In our case, this can be seen as oscillations of the system around one of the critical points and random jumps to other critical point and vice versa in unpredictable fashion. Of course, the dynamics of equations (1) driven by external forces is much more complex than that of Duffing's system because (1) is more than a nonlinear oscillator but a system possesing complex spatio-temporal structures.

IX.- Conclusions.

We have studied the solitons that result from the solution of the torsional equations of Yakushevich for the DNA.

Our research shows that the most important solitons are those of type (9) because they are the only strictly stable ones and they play the part of building blocks to form more complex structures. It is surprising that this solitons have received very little attention in current literature.

Besides that, other works dedicated to Yakushevich's model consider only the simplified case ($I_0 = 0$), which we show to have important dynamical differences with the exact and more realistic model.

We have shown that all the solitons in the exact model have long range interaction. This phenomenon can be of particular interest in the regulation of biological processes like replication and transcription of DNA, because the existence of open states in one place of the chain can influence the dynamics of other distant open states. Furthermore, a soliton propagating through the chain can contribute to its opening helping these processes.

The original Yakushevich system is structurally unstable under external torques. When they act, the critical points stop being degenerated, which changes the range of the soliton interaction. For a given relation between the torques, the equilibrium points can bifurcate and instead of one appear three, one unstable and two stable, something like a Thom's catastrophe

All this situation generates a series of complex structures. It is possible that torques are present at all times due to the normal torsion of the spiral chain In that case, the system (40) proposed by us is much more adapted to the reeal situation than system (1), and also it is structurally more stable.

The dynamics and interactions of the solitons axisting in these equations are extremely rich. We have developed a qualitative theory to describe it.. If the system is perturbed by a periodical force then chaotical dynamics might appear.

Acknowledgments

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Figure Captions.

Figure 1. Critical points of $V(\varphi_1, \varphi_2)$ and phase plane trajectories corresponding to solitonic solutions of (2).

Figure 2. Solitonic solution of equations (2) with properties (9.1).

Figure 3. Solitonic solution of equations (2) with properties (9.2).

Figure 4. Solitonic solution of equations (2) with properties (9.3).

Figure 5. Solitonic solution of equations (2) with properties (10.1).

Figure 6. Solitonic solution of equations (2) with properties (10.2.1).

Figure 7. Solitonic solution of equations (2) with properties (10.2.2).

Figure 8. Solitonic solution of equations (2) with properties (10.2.3).

Figure 9. Bifurcation diagram for system (40).

Figure 10. Small solitonic solution (baby soliton) in perturbed system with $h_1 = -h_2$.

Figure 11. Repulsive force due to chain interaction between solitons with chain charge of different sign.

Figure 12. Kink-antikink stable state under external forces due to chain interaction $h_1 = -h_2$.

Figure 13. Kink-kink stable state under external forces due to chain interaction $h_1 = h_2$.

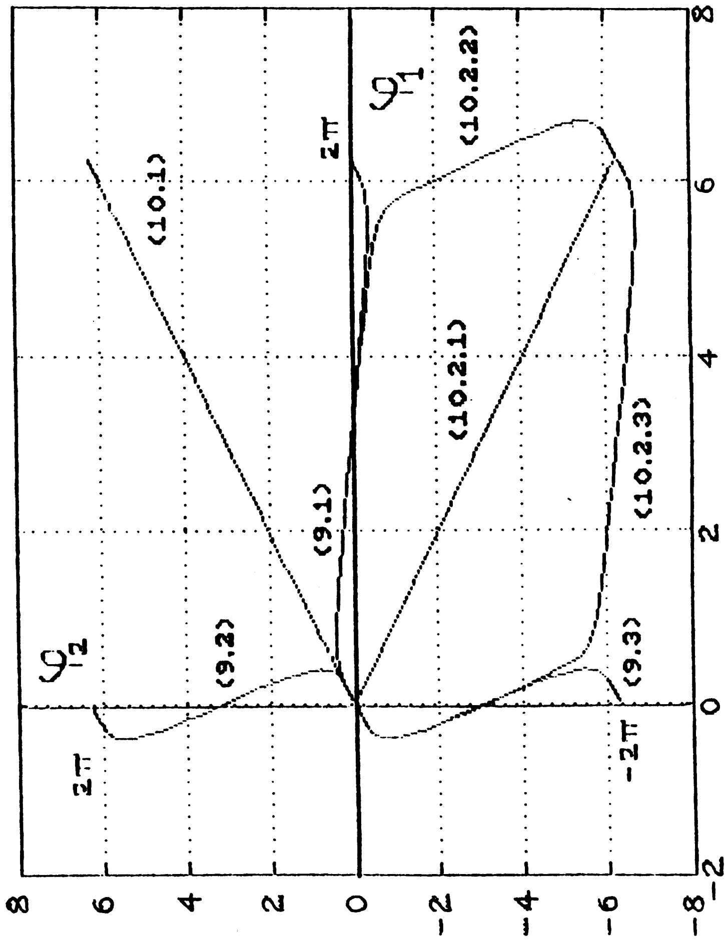


Fig.1

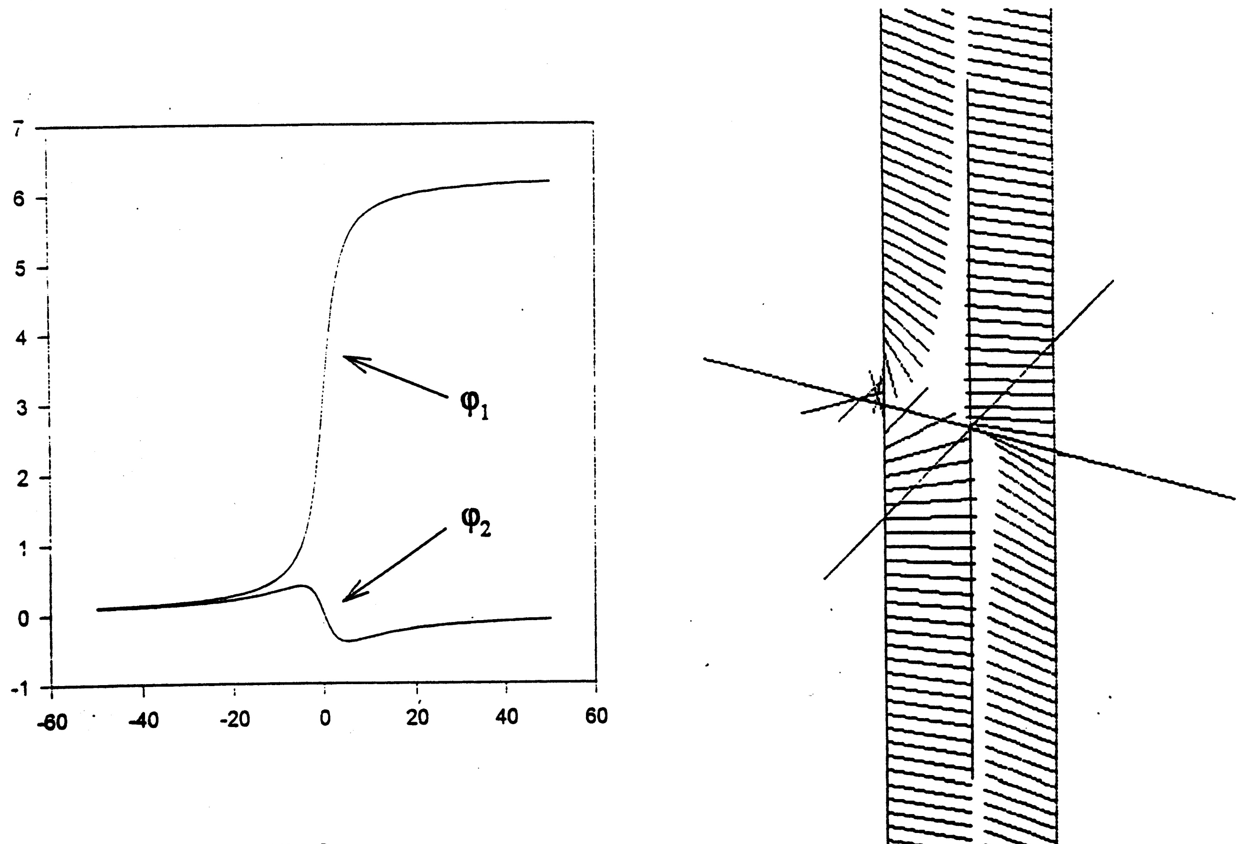


Fig.2

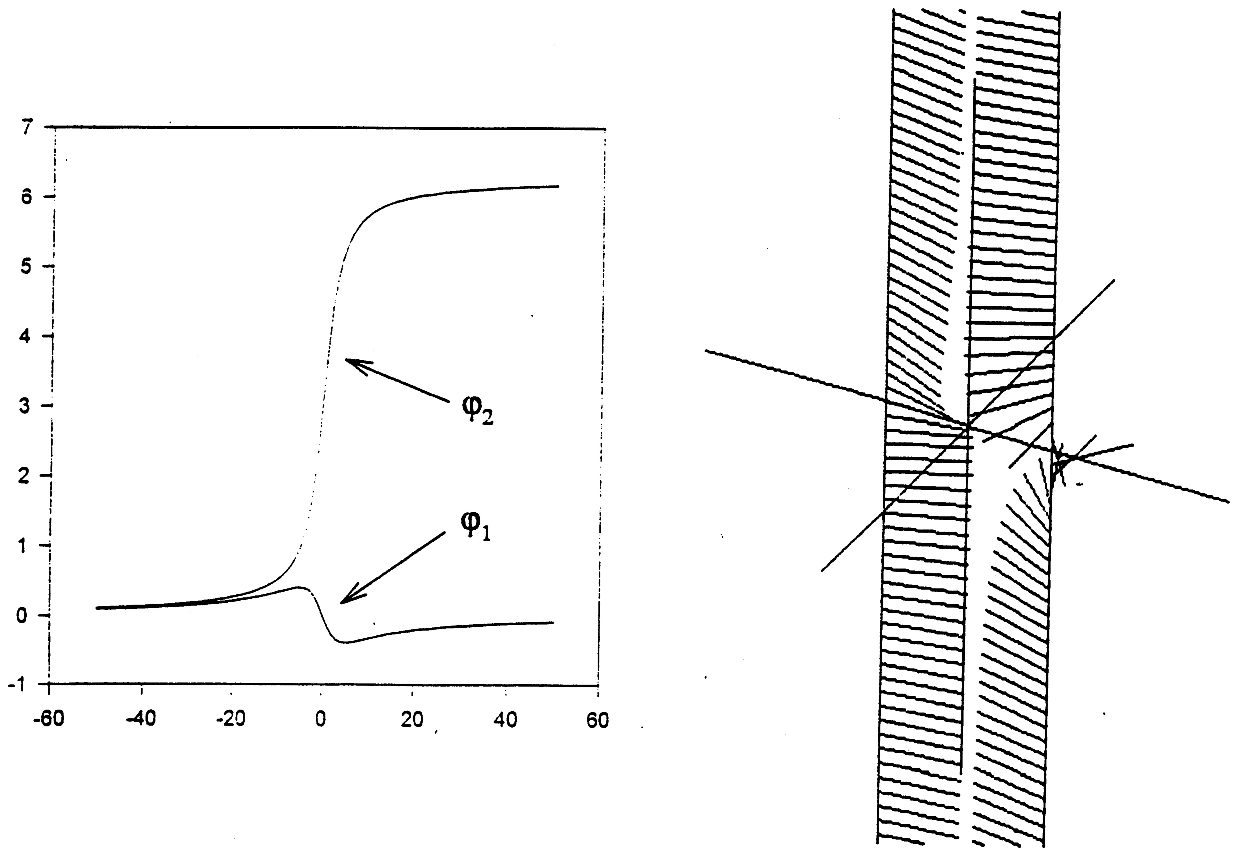
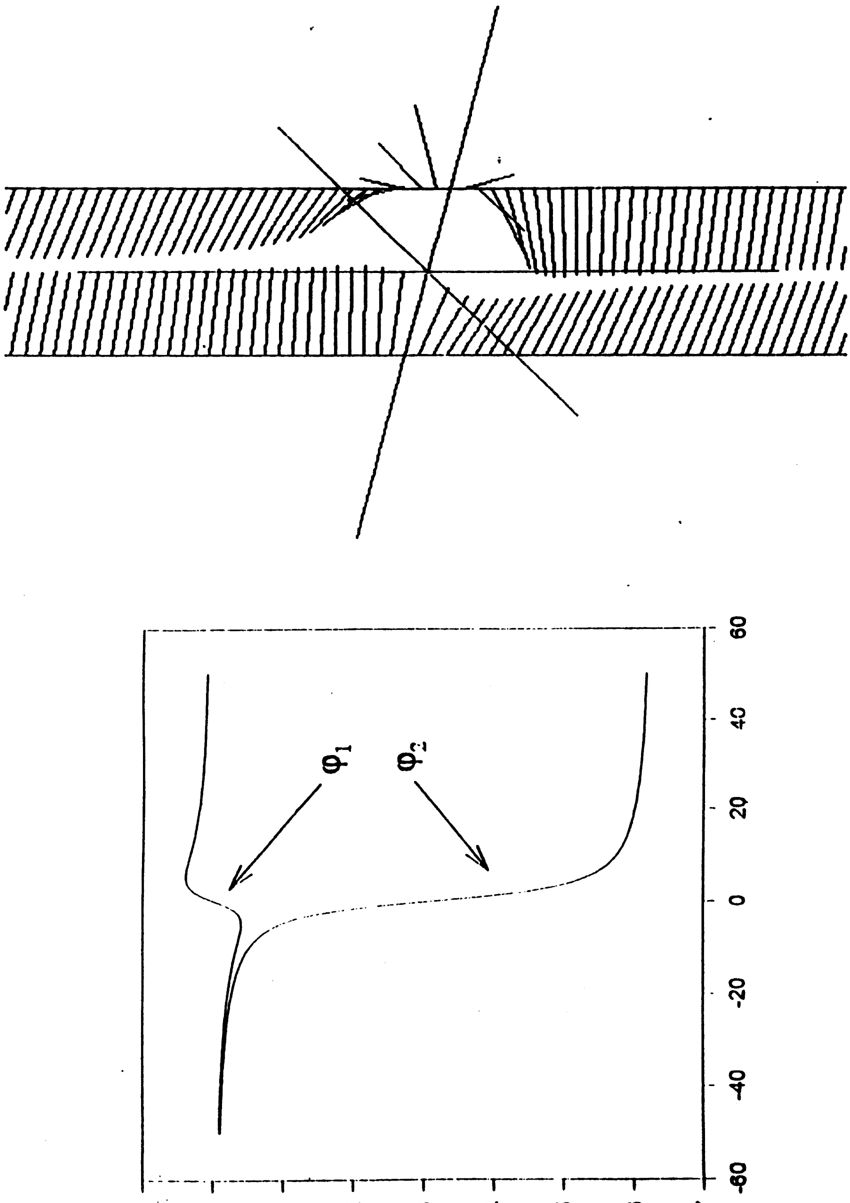


Fig.3



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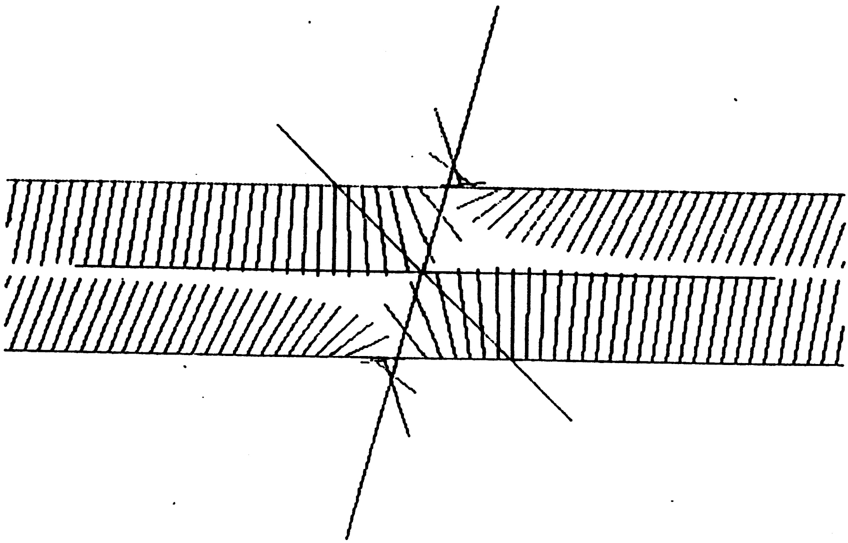


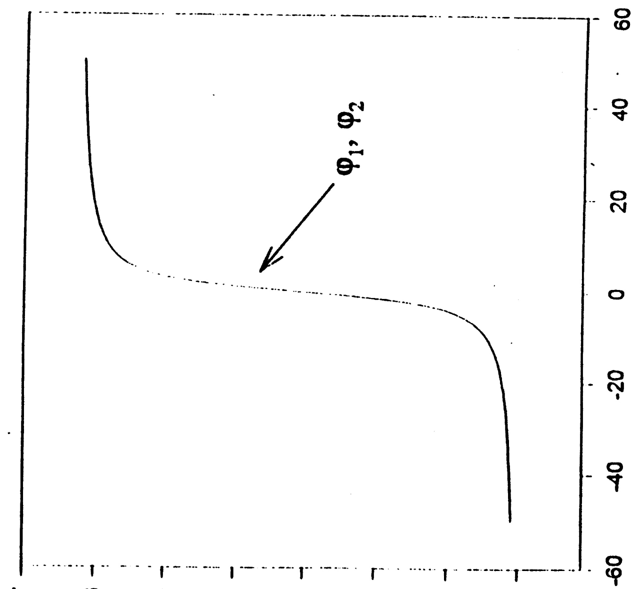


Fig.5

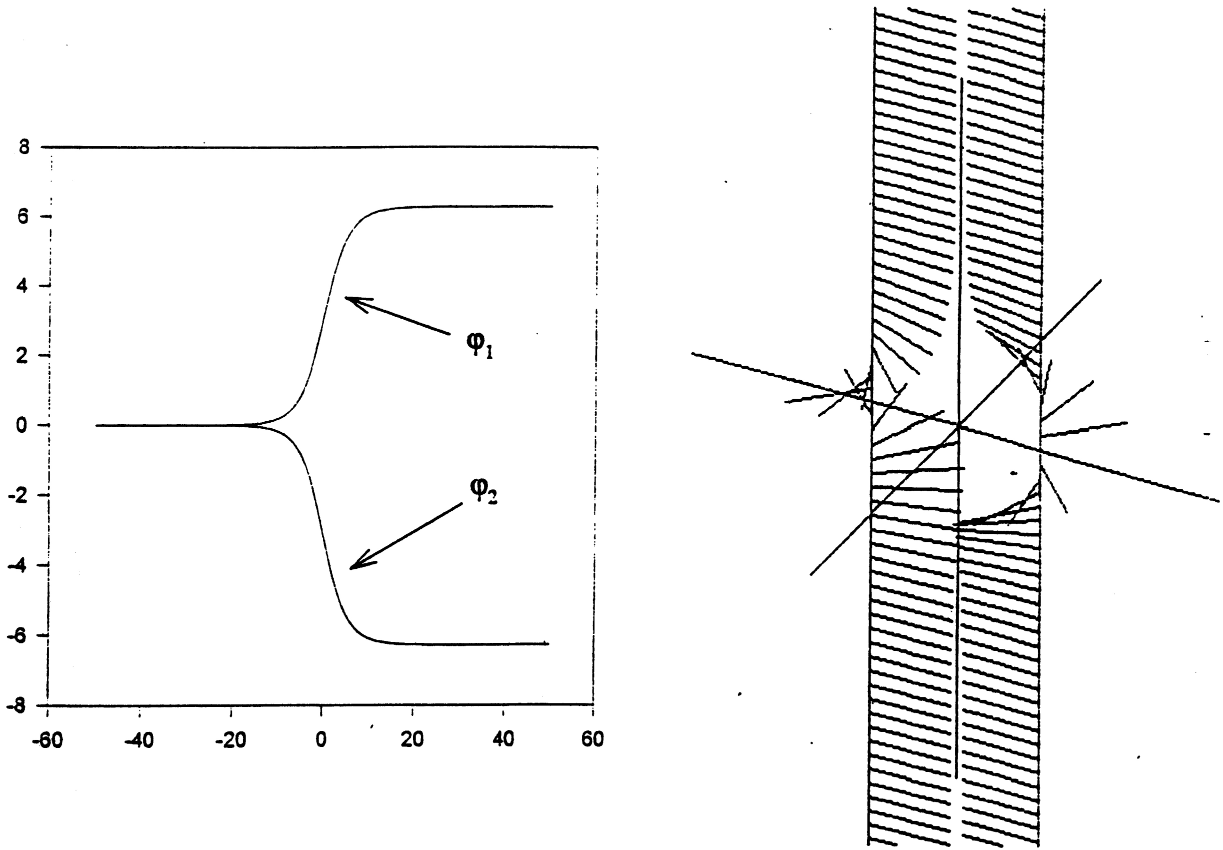


Fig.6

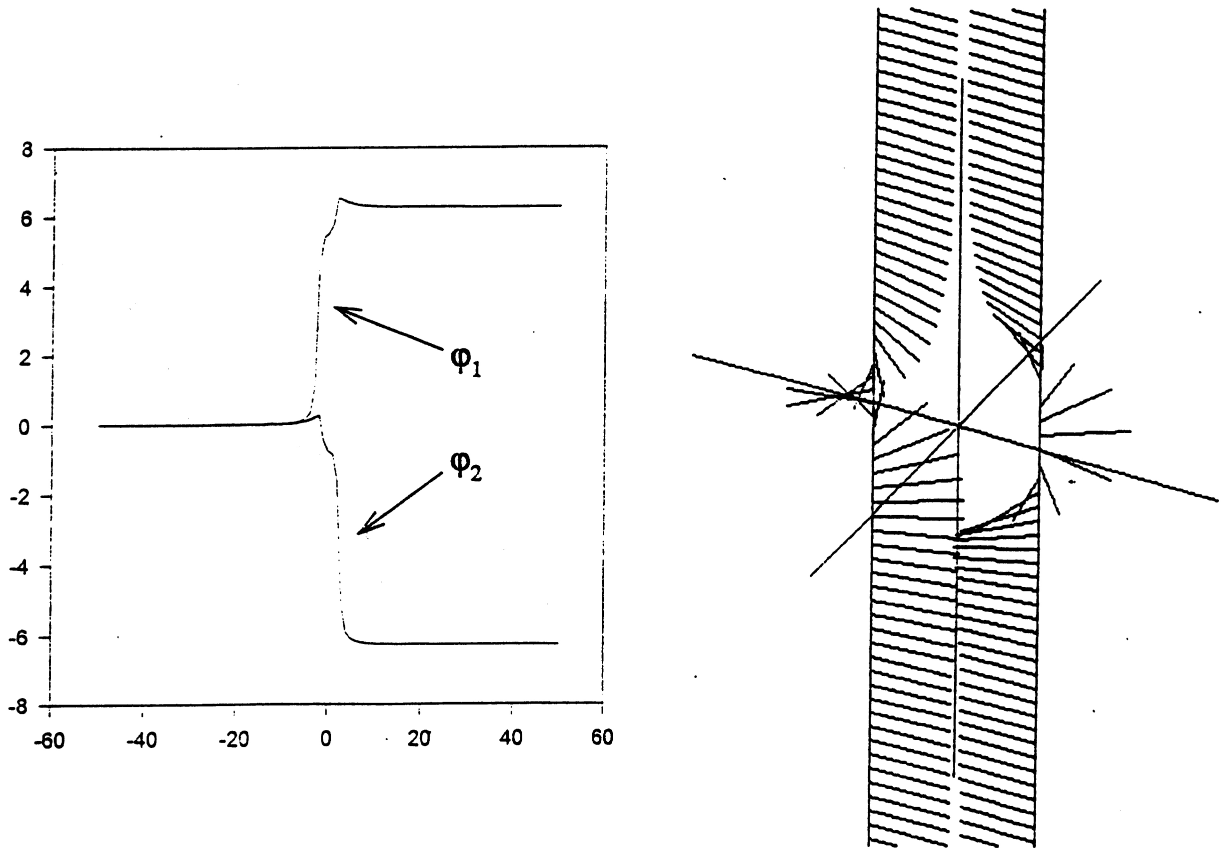


Fig.7

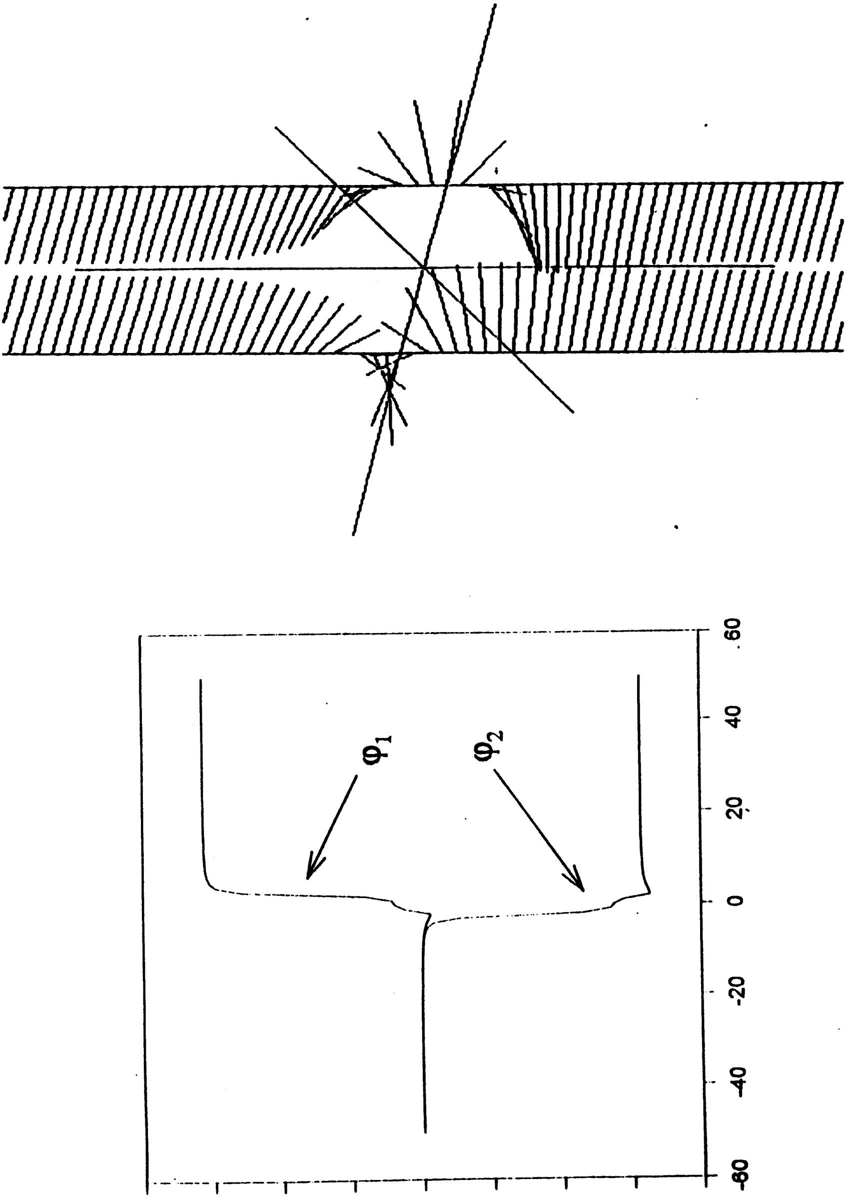


Fig.8

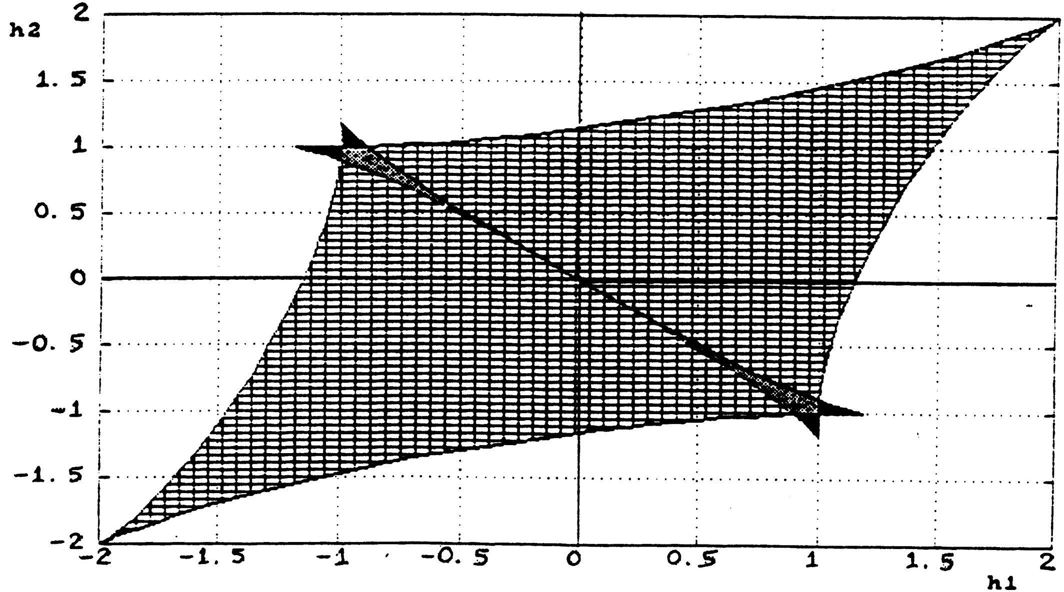
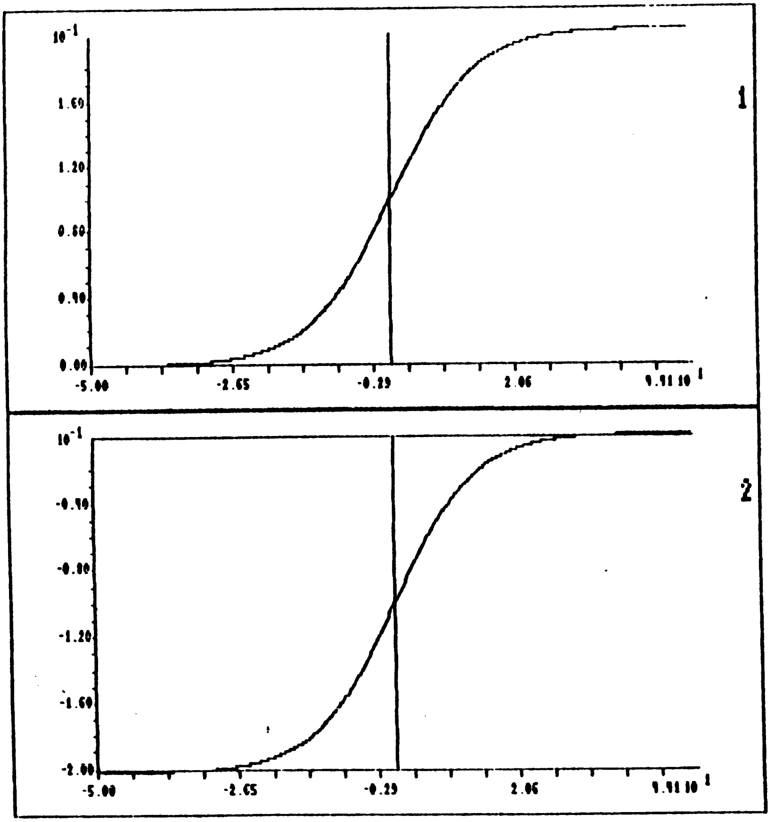


Fig.9



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1.60
1.20
0.80
0.40
0.00
-5.00
-2.65
-0.29
2.06
2
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-0.29
2.06

Fig.10

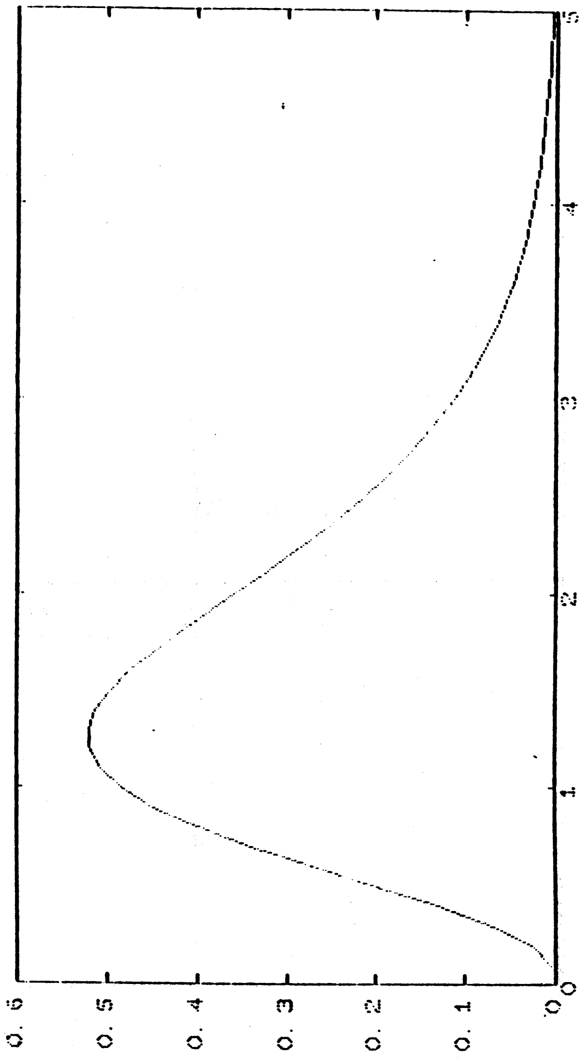

Fig.11

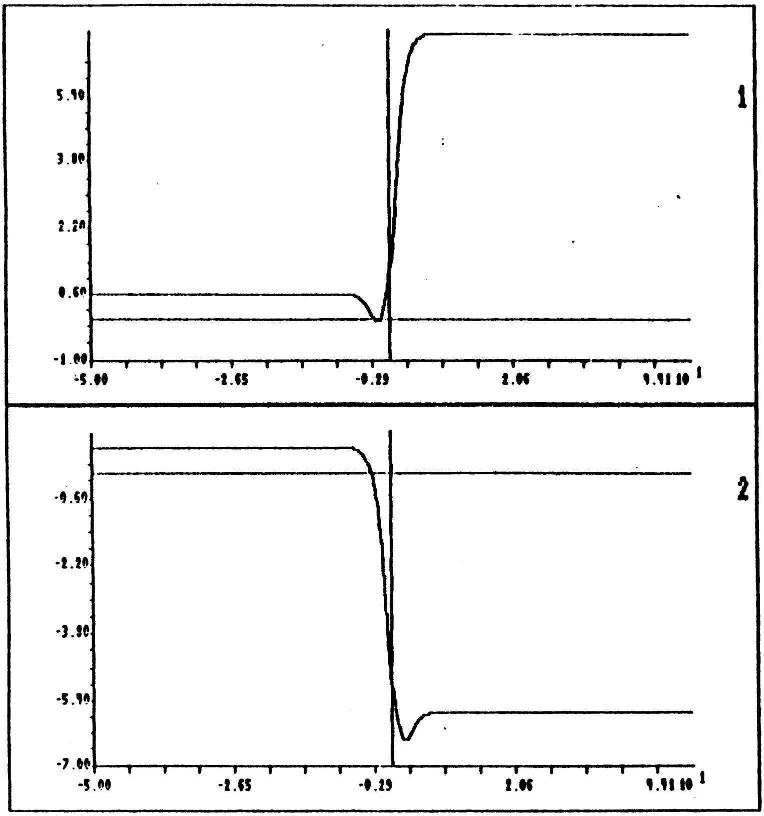

Fig.12

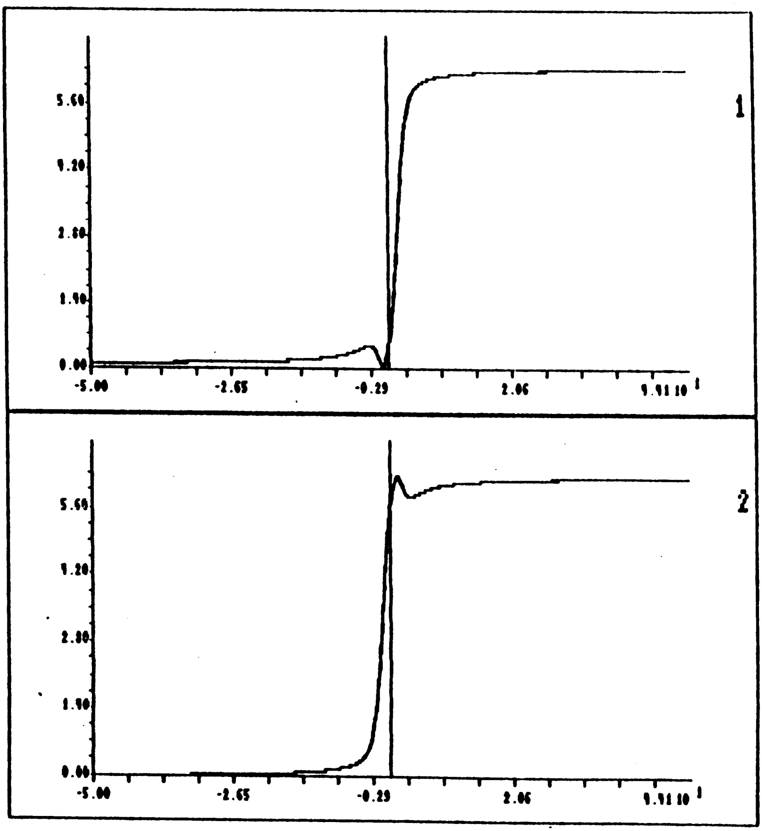

Fig.13