Nonlinear Polarisationoscillations in a Biophysical Model-System I: Internal Dynamics

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Nonlinear Polarisationoscillations

To describe a metastable electrical dipole state in a biological system, Fröhlich suggested a nonlinear model potential. In this paper we investigate a system of two such dipoles coupled by a dipole-dipole interaction. Mathematically this model is described by two coupled nonlinear differential equations. In the investigation of the dynamics of the system we distinguish three solution types of the equations of motion.

I. The Model

In 1968 Fröhlich has suggested that long wave-length electric vibrations are very strongly and coherently excited in active biological systems. Furthermore, if such a long wave electric mode interacts with the elastic field of the system, a meta-stable state with a permanent polarization can be stabilized [1, 2]. Thus the nonlinear coupling of elastic and polar modes and an additional energy supply may evoke a quasi-ferroelectric behaviour, *i.e.* the activation of a high dipole moment.

These suggestions have received theoretical support through some single model calculations [2, 4]. In the "high polarization model" the possibility of the existence of metastable highly polarized state has been shown [3], whereby a nonlinear potential of the form

$$U(P) = \frac{m}{e^2} \left(\frac{1}{2} WP^2 - \frac{1}{C} CP^4 + \frac{1}{6} DP^6 \right) \quad (1)$$

has been derived.

With W, C, $D > 0$, where $P = e\,r$ represents the electrical dipole of size r, charges $\pm e$ and mass m. $\sqrt{W}$ is the harmonic eigenfrequency of the dipole. C, D are positive constants representing the non-linear part of the potential. For symmetry reasons, there are only even powers of P in $U(P)$ (vid. in Fig. 1).

In the present paper Fröhlich's model has been extended to a system of two interacting dipoles, P_1

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and P_2. Both of them have a nonlinear potential of the form (1) and they are coupled by a dipole-dipole interaction $P_1 P_2/\varepsilon R^2$. ε is the dielectric constant, R is the distance between the two dipoles. The frequency dependence of ε has been taken into account by Genzel in a model of linearly coupled harmonic dipole oscillators [5].

In this investigation we only want to discuss the undamped behaviour of the model, *i.e.* conservative system. The influence of external fields and of loss processes will be discussed in a forthcoming paper [6].

The equations of motions of this system can be derived from the Lagrangian function L, it reads

$$
\begin{aligned}
L = &\frac{1}{2} \frac{m}{e^2} (\dot{P}_1^2 + \dot{P}_2^2) - \frac{1}{2} \frac{m}{e^2} W (P_1^2 + P_2^2) \\
&+ \frac{1}{4} \frac{m}{e^2} C (P_1^4 + P_2^4) - \frac{1}{6} \frac{m}{e^2} D (P_1^6 + P_2^6) \\
&- \frac{P_1 P_2}{\varepsilon R^3}
\end{aligned}
\quad (2)
$$

from which the following equations of motion

$$\ddot{P}_1 + WP_1 - CP_1^3 + DP_1^5 + \frac{P_2}{R^3} = 0 , \quad (3)$$

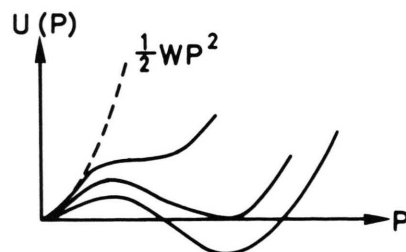Fig. 1. Forms of the model potential (1) depending on different constants W, C, D. – – – – harmonic part.

$$\ddot{P}_2 + WP_2 - CP_2 + DP_2^5 + \frac{P_1}{R_3} = 0 , \qquad (4)$$

can be deduced. P and R have been transformed to new qualities, where m/e^2 and ε are included.

II. Steady States and Stability Investigations

Setting all time derivations of Eqs. (3) and (4) to zero we arrive at the steady states equations:

$$WP_1 - CP_1^3 + DP_1^5 + \frac{P_2}{R^3} = 0 , \qquad (5)$$

$$WP_2 - CP_2^3 + DP_2^5 + \frac{P_1}{R^3} = 0 . \qquad (6)$$

Eqs. (5), (6) are both of 5. order, in P_1 and P_2, respectively, therefore the system can have up to 25 steady states [7].

We restrict ourselves to an analytic investigation of the special case,

$$P_1 = \sigma_P P_2 = P , \qquad (7)$$

where $\sigma_P = \pm 1$, corresponding to a parallel or anti-parallel dipole configuration. With (7) the set of Eqs. (5) and (6) is reduced to

$$WP - CP^3 + DP^5 + \frac{\sigma_P P}{R^3} = 0 \qquad (8)$$

leading to the steady state solutions:

$$P_\alpha = 0 , \qquad (9)$$

$$P_{\beta/\gamma}^{\sigma_P} = \sqrt{\frac{C}{2D}(1 \pm \sqrt{1 - \lambda^*})} \qquad (10)$$
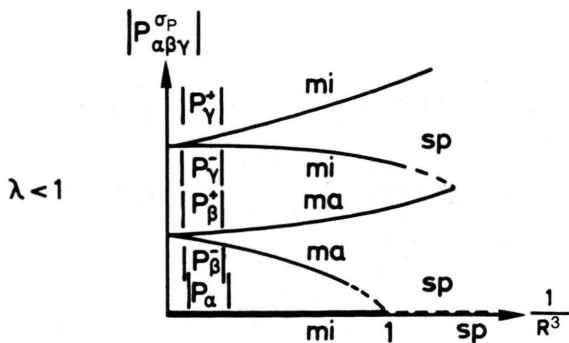

Fig. 2. Analytically calculated steady states $P_1 = P_2 = P_\alpha = 0$ and $P_1 = \sigma_P P_2 = P_{\beta,\gamma}^{\sigma_P}$ and their stability as a function of the distance parameter R. —— minimum (mi), stable; maximum (ma), unstable; - - - - saddlepoint (sp), unstable.

with

$$\lambda^* = \frac{4D}{C^2}\left(W + \sigma_P \frac{1}{R^3}\right) . \qquad (11)$$

From Eq. (10) it is obvious that only for $\lambda^* \leq 1$ we have a metastable state with not vanishing permanent dipole moment $P_\gamma^{\sigma_P} > 0$. Therefore in the following we restrict ourselves to the case $\lambda < 1$ where

$$\lambda = \frac{4D}{C^2} W . \qquad (12)$$

Because only in this case we have for both values ± 1 of σ_P possible not vanishing permanent dipoles $P_\gamma^{\sigma_P} > 0$.

To investigate the stability of the steady states we have to discuss the potential energy $W(P_1, P_2)$. The result is shown in Fig. 2. It turns out that at least three steady states are stable.

III. Dynamics of the Model

We want to discuss the dynamics of Eqs. (3), (4) by distinguishing three cases:

III.1. Quasilinear case

Introducing a linear transformation

$$P_1(t) = P_{10} + X_1(t) , \qquad (13)$$

$$P_2(t) = P_{20} + X_2(t) , \qquad (14)$$

where (P_{10}, P_{20}) is a minimum steady state, we get a set of equations in $X_1(t)$ and $X_2(t)$ [7]:

$$\ddot{X}_1 + \alpha_1 X_1 + \frac{X_2}{R^3} + F_1(X_1) = 0 , \qquad (15)$$

$$\ddot{X}_1 + \beta_1 X_2 + \frac{X_1}{R^3} + F_2(X_2) = 0 . \qquad (16)$$

α_1, β_1 are constants:

$$\alpha_1 = W - 3CP_{10}^2 + 5DP_{10}^4 , \qquad (17)$$

$$\beta_1 = W - 3CP_{20}^2 + 5DP_{20}^4 . \qquad (18)$$

$F_1(X_1)$ and $F_2(X_2)$ are perturbation functions containing nonlinear terms in X_1 and X_2. For small values $X_1(t)$ and $X_2(t)$ the quasi-linear Eqs. (15) and (16) can be solved approximately with the Krylov-Bogoliubov-Mitropolsky method [8]. Near a minimum (P_{10}, P_{20}) $P_{10}, P_{20} \neq 0$, this method as-
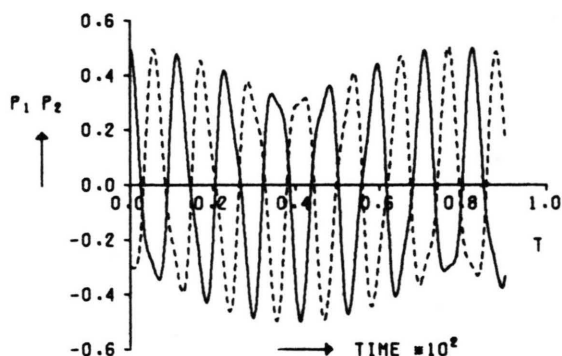
Fig. 3. Oscillation diagram. Polarisation P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the quasilinear case.

sumes a solution of the form:

$$X_1(t) = a_1 \cos(\omega_1 t + \varphi_1)$$
$$+ a_2 \cos(\omega_2 t + \varphi_2(t)), \qquad (19)$$

$$X_2(t) = \alpha_1 \cos(\omega_1 t + \varphi_1)$$
$$- a_2 \cos(\omega_2 t + \varphi_2(t)), \qquad (20)$$

where a_1, a_2 are constants, ω_1, ω_2 áre linear eigenfrequencies of the system, φ_1 is a constant phase and $\varphi_2(t)$ is a harmonically variing phase function.

In summarizing this approximation shows that the influence of nonlinearities leads to a periodic change of the momentary frequency $\omega_2 + \dot{\varphi}_2(t)$. On the average the nonlinearities do not change the harmonic behaviour. An example is given in Fig. 3. In this case the oscillations repeat after $t = 83$. This shows the conformity with the approximative analytic solution above.
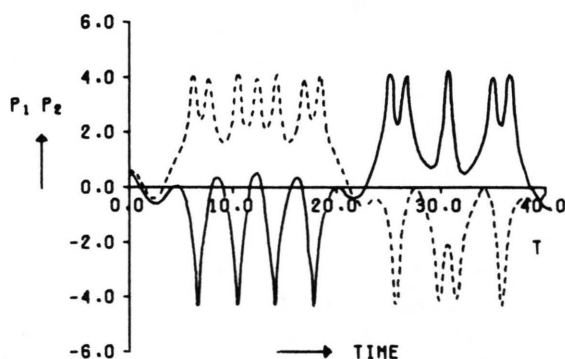
III.2. General case

We solve the equations of motions (3) and (4) with the computer in a time interval $(0, T)$. It turns out that the solutions exhibit an extreme sensitivity to the initial conditions [7]. In our case four different types of solutions have been found with respect to the initial conditions.

a) Chaotic behaviour

In the interval $(0, T)$ the solutions $P_1(t)$ and $P_2(t)$ are nonperiodic and bounded (vid. Fig. 4). Necessary is a strong coupling of the dipoles, which has been achieved by small values of the distance parameter R. The system exhibits a "flip" behaviour. The dipoles P_1 and P_2 interchange their position after a time-interval $\Delta t \approx 20$.

b) Chaotic-periodic behaviour

One dipole shows a chaotic, the other dipole a periodic behaviour (vid. Fig. 5). Perturbations may occur because of the interaction energy.

c) Periodic-constant behaviour

Both dipoles are oscillating periodically. The relation of their amplitudes is about 1 to 10. This means that one dipole is nearly constant compared with the other one. Again perturbations in the time behaviour are caused by the interaction. A typical example is shown in Fig. 6.

d) Periodic behaviour

Both dipoles are oscillating periodically and have amplitudes within the same order of magnitude, which can be seen from Fig. 7.
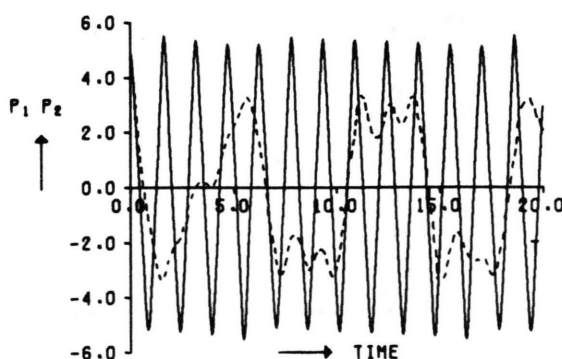

Fig. 4. Oscillation diagram. Polarization P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the chaotic case.

Fig. 5. Oscillation diagram. Polarization P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the chaotic periodic case.
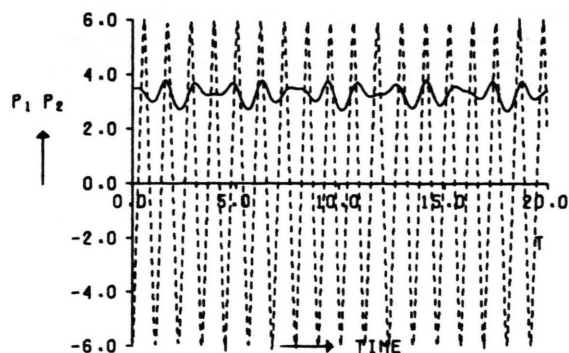
Fig. 6. Oscillation diagram. Polarization P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the periodic-constant case.
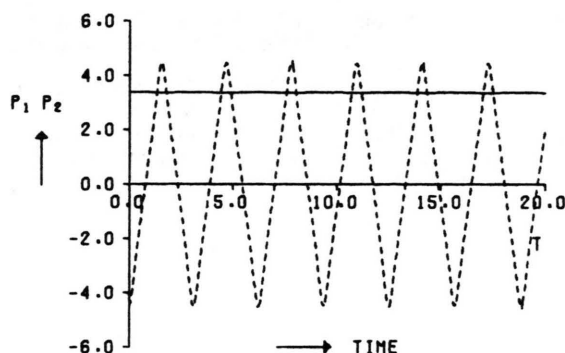

Fig. 8. Oscillation diagram. Polarization P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the quasi-discoupled case.
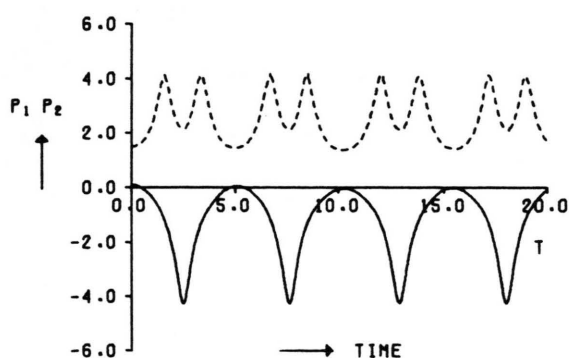

Fig. 7. Oscillation diagram. Polarization P_1, P_2 as a function of time t. Computersolution of the equations of motion (3) and (4) for the periodic case.

III.3. Quasi decoupled case

For large values of the distance parameter R the interaction energy $P_1 P_2/R^3$ becomes very small. This leads to almost autonomous behaviour of the two nearly decoupled dipoles P_1 and P_2, respectively (vid. Fig. 8). The triangle like oscillation of the dipole P_2 shows the high nonlinearity of the system.

IV. Summary and Outlook

A significant result of our investigations is the occurrence of solutions, which are asymmetric with respect to the polarization P_1 and P_2. This is a nonlinear effect, since the equations of motion of the model are symmetric in P_1 and P_2. In our model this asymmetry can either be permanent or time dependent *i.e.* similar to a switch effect. This energy exchange may be of importance for biological systems.

If, for example, two biological units approach one another, one of them may be activated in a highly polar state which means, that energy is predominantly localized in one single degree of freedom of the entire system.

Furthermore, the model has shown a high sensitivity to initial conditions leading to different types of solution. This means, that small external perturbations can create a structural change in the system's behaviour, *e.g.* from chaotic to periodic behaviour. This effect may be of some importance for the extreme sensitivity of biological systems to electromagnetic radiation [9, 10].

To discuss the influence of an external stimulus (*e.g.* electric field) we have extended the conservative model system towards a more realistic situation. This has been achieved by introducing both, a linear damping term and an external drive. In a forthcoming paper we will present some results of a quantitative investigation of the generalized model [6]. Though our models are rather crude approximations they exhibit a very specific behaviour which might be important for some typical phenomena known from biological systems.

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