Nonlinear Polarisationoscillations in a Biophysical Model System II: External Dynamics

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Nonlinear Polarisationoscillations

To describe a metastable electric dipole state in a biological system, Fröhlich suggested a nonlinear model potential. In this paper we investigate a system of two nonlinear dipoles, which are coupled by a dipole-dipole interaction. We apply an external field and add linear damping terms. The external drive leads to a phase-locking of the dipoles. Mathematically, the system corresponds to an externally driven anharmonic oscillator with damping. We investigate the system of coupled oscillators and look for the stable and metastable solutions as a function of the internal and external parameters.

Introduction

In recent years considerable attention has been given to understanding both the stability of biological systems and their interactions with non-ionizing electromagnetic waves. These problems have gained increasing interest both, through rather exciting experimental results and through theoretical considerations [1].

As early as 1967 Fröhlich (vid. ref. [1]) emphasized that biological systems exhibit a relative stability for some modes of behaviour. In their active state (*in vivo*) these modes remain very far from thermal equilibrium. To give an interpretation of such a specific behaviour, Fröhlich has suggested that both, coherent oscillations and highly polarized metastable states should be of great importance in biological membranes and in other biological systems as well. Both concepts have been supported by some rather simple model calculations [1].

The aim of the present paper is to discuss further some consequences which result from an extension of Fröhlich's second model, the high polarization model. Furthermore, the idea of making such simple models is suggested by the enormous complexity, which characterizes biological systems. With the aid of models it might be possible to find a description of those mechanisms which are responsible for both the internal function of the system and its interaction with an external field.

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1. The Model

In a recently published paper [2] (henceforth referred to as I) we have investigated a system of two interacting dipoles, P_1 and P_2. Both of them are governed by a nonlinear potential of the form [1]

$$U(P) = \frac{m}{e^2}\left(\frac{1}{2}\,W P^2 - \frac{1}{4}\,C P^4 + \frac{1}{6}\,D P^6\right). \quad (1)$$

In addition, they are coupled by a dipole-dipole interaction of the well-known form

$$\frac{P_1 P_2}{\varepsilon R^3}. \quad (2)$$

$P = e\,r$ represents a dipole of size r, $\pm e$ are charges and m is the mass of the oscillators. R is the distance between the two dipoles. ε is the dielectric constant.

In I we have investigated the internal dynamics of the system, which have been described by a set of two coupled, nonlinear differential equations

$$\ddot{P}_1 + W P_1 - C P_1^3 + D P_1^5 + \frac{P_2}{\varepsilon R^3} = 0 \quad (3\,a)$$

$$\ddot{P}_2 + W P_2 - C P_2^3 + D P_2^5 + \frac{P_1}{\varepsilon R^3} = 0 \quad (3\,b)$$

where P and R are transformed quantities, including the parameter m/e^2. The aim of the present paper is to investigate the influence of an external electric field $F = F_0 \cos \omega\, t$ on the dipole system. F_0 is the amplitude and ω the frequency of the external stimulus.

In order to make our system more realistic and for stability reasons we have to introduce energy dissipating processes. A possible choice is friction of

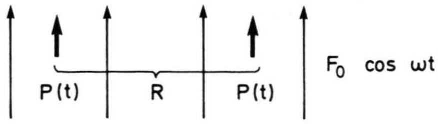

Fig. 1. Complete phase-locking of the two induced dipoles due to the external field $F_0 \cos \omega t$, $P_1(t) = P_2(t) = P(t)$. P_1 and P_2 are assumed to be parallel to the external field.

the Stokes type, *i.e.* a term, which is proportional to $\dot{P}$. This choice seems reasonable, since dipole oscillations are coupled with mechanical oscillations of the carriers, which in turn lead to frictional losses into the surrounding medium. Because of the dissipation we have to regard the dipoles P_1, P_2 as being induced by the external field F. We assume furthermore the dipoles P_1, P_2 to be parallel to the external field F.

Mathematically, we describe the energy dissipation by additional linear terms, $K\dot{P}_1$ and $K\dot{P}_2$ in the equations of motion (Eqn. 3a, b). K is a parameter determining the strength of energy dissipation. For reasons of symmetry, we take the same constant for both dipoles, P_1 and P_2, respectively.

With the above extensions the equations of motion read

$$\ddot{P}_1 + K\dot{P}_1 + WP_1 - CP_1^3 + DP_1^5 + \frac{P_2}{\varepsilon R^3} = F_0 \cos \omega t \tag{4}$$

$$\ddot{P}_2 + K\dot{P}_2 + WP_2 - CP_2^3 + DP_2^5 + \frac{P_1}{\varepsilon R^3} = F_0 \cos \omega t\,. \tag{5}$$

According to a theorem of Trefftz [3], equations of the type (4, 5) exhibit periodic sulutions after the transients have died out. The period is either equal to the external period $T = 2\pi/\omega$ or to an integer multiple or submultiple of T, *i.e.* subharmonics or superharmonics of the external field, respectively.

In the following discussion, we restrict ourselves to the case, where the external drive leads to a complete in-phase oscillation of the two dipoles $P_1(t)$ and $P_2(t)$. We describe this behaviour with the relation

$$P_1(t) = P_2(t) = P(t)\,. \tag{6}$$

Graphically, this assumption is shown in Fig. 1

With Eqn. (6) the set of differential equations (4, 5) is reduced to one single differential equation for $P(t)$. It reads

$$\ddot{P} + K\dot{P} + \left(W + \frac{1}{\varepsilon R^3}\right) P - CP^3 + DP^5 = F_0 \cos \omega t\,. \tag{7}$$

In the special case $D = 0$, Eqn. (7) leads to the well-known equation of the forced Duffing oscillator with friction [4].

2. Steady States

With the restriction $K = 0$ and without an external field (*i.e.* $F_0 = 0$), a potential of the following form can be derived for the equation of motion of the dipoles:

$$U(P) = \frac{1}{2}\left(W + \frac{1}{\varepsilon R^3}\right) P^2 - \frac{1}{4} CP^4 + \frac{1}{6} DP^6. \tag{8}$$

The detailed shape of the potential $U(P)$ is strongly depending on the distance parameter R. Some possible and most important realizations are given in Fig. 2.

To calculate the steady states of Eqn. (7), *i.e.* $\ddot{P}(t) = 0$ for $K, F_0 = 0$, we can determine the solutions of the equation

$$\frac{\partial}{\partial P} U(P) = 0\,. \tag{8'}$$

The solutions read

$$P_0 = 0 \tag{9}$$

$$P_{max} = \left\{\frac{c}{2D}\left(1 - \sqrt{1 - \frac{4D}{C^2}\omega_0^2}\right)\right\}^{1/2} \tag{10}$$

$$P_{min} = \left\{\frac{c}{2D}\left(1 + \sqrt{1 - \frac{4D}{C^2}\omega_0^2}\right)\right\}^{1/2} \tag{11}$$

where we have introduced the abbreviation ω_0^2,

$$\omega_0^2 = W + \frac{1}{\varepsilon R^3} \tag{12}$$

being the square of a frequency.

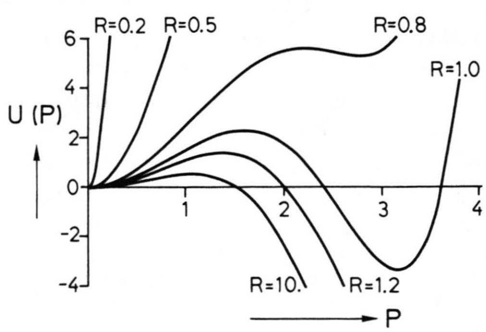

Fig. 2. Potential $U(P)$ of the system as a function of the polarization P for different values of the distance parameter R. $W = 1$, $C = 1$, $D = 0.08$.

According to Fröhlich [1], we are interested in the excitation of metastable dipole states. A possible realization is given by the set of parameters $W = 1$, $C = 1$, $D = 0.08$, $R = 0.8$ (vid. Fig. 2). In this case the steady states P_0 and P_{min} correspond to minima of the potential, whereas P_{max} is a maximum.

3. Approximative Solutions of the Equations of Motion

The solutions $P(t)$ of Eqn. (7) are periodic (Theorem of Trefftz [3]), if transients are neglected or if the solutions have built up. Consequently, $P(t)$ can be expanded in a series of harmonics, sub- and superharmonics. It reads

$$\begin{aligned} P(t) = P_{const} &+ A_1 \cos \omega t + A_2 \cos 2\omega t + \dots \\ &+ A_{\frac{1}{2}} \cos \frac{\omega}{2} t + \dots \\ &+ B_1 \sin \omega t + B_2 \sin 2\omega t + \dots \\ &+ B_{\frac{1}{2}} \sin \frac{\omega}{2} t + \dots \, . \end{aligned} \tag{13}$$

In the case that the solution $P(t)$ is bounded to a small surrounding of a minimum P_0 or P_{min}, we will calculate it with the method of Harmonic Balance [5]*. This method assumes that the dominating solution is almost harmonic, therefore sub- and superharmonics are neglected in a first approximation in calculating the coefficients P_{const}, A_1 and B_1.

3.1 *Harmonic balance for the minimum $P_0 = 0$*

Presupposing that the solution $P(t)$ is restricted to $|P(t)| < P_{max}$ (vid. Fig. 3), we make the ansatz

$$P(t) = A \cos \omega t + B \sin \omega t \, . \tag{14}$$

For reasons of symmetry, P_{const} is set equal to zero. To calculate the coefficients A and B we insert Eqn. (14) into the equation of motion (7). With the definition

$$r^2 = A^2 + B^2 \tag{15}$$

(r is the amplitude of oscillation) and with the formulas of the appendix we get after a consequent

* A comparison of the results of the Harmonic Balance approximation with numerical calculations shows a supprisingly good correspondence between the two methods [6].

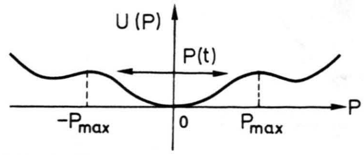

Fig. 3. Potential $U(P)$ as a function of the polarization P. The time-dependent polarization $P = P(t)$ is restricted to $-P_{max} < P(t) < P_{max}$, *i.e.* to an oscillation around the minimum $P = P_0$.

neglection of sub- and superharmonic terms [6]

$$-A\omega^2 + KB\omega + A\omega_0^2 - \frac{3}{4} Cr^2 A + \frac{5}{8} DAr^4 = F_0 \tag{16}$$

$$-B\omega^2 - KA\omega + B\omega_0^2 - \frac{3}{4} Cr^2 B + \frac{5}{8} DBr^4 = 0 \tag{17}$$

where the coefficients of the terms containing $\cos \omega t$ and $\sin \omega t$ have been equated to zero separately.

With the definition of an effective frequency $\tilde{\omega}(r)$

$$\tilde{\omega}^2(r) = \tilde{\omega}_0^2 - \frac{3}{4} r^2 C + \frac{5}{8} r^4 D \tag{18}$$

we can reduce Eqns. (16, 17) to

$$(-\omega^2 + \tilde{\omega}^2(r))\, A + KB\omega = F_0 \tag{19}$$

$$(-\omega^2 + \tilde{\omega}^2(r))\, B - KA\omega = 0 \, . \tag{20}$$

These equations correspond to the equations of driven harmonic oscillators, the frequency of which has been replaced by an effective one, $\tilde{\omega}$. Summing up the squares of Eqns. (19, 20), we arive at an implicit relation for the resonance amplitude $r(K, F_0, \omega)$ of the forced oscillators. It reads

$$r^2([-\omega^2 + \tilde{\omega}^2(r)]^2 + K^2\omega^2) = F_0^2 \, . \tag{21}$$

Instead of a discussion of the function $r(K, F_0, \omega)$ it is more convenient to discuss the invers function $\omega(K, F_0, r)$, which is deduced from Eqn. (21) in the following form

$$\omega^2 \pm = \tilde{\omega}^2(r) - \frac{K^2}{2} \pm \sqrt{\frac{K^4}{4} - K^2\tilde{\omega}^2(r) + \frac{F_0^2}{r^2}} \, . \tag{22}$$

For physical reasons, only real values $\omega_\pm^2 \geqq 0$ are allowed in Eqn. (22). The shape of the function $r(K, F_0, \omega)$ is given in the lower part of Fig. 5.

3.2 *Harmonic balance for the minima P_{min}*

If $P(t)$ fulfills the condition $P_{max} < P(t)$ (vid. Fig. 4), we can make the ansatz

$$P(t) = P_{min} + P'_{const} + A' \cos \omega t + B' \sin \omega t \, . \tag{23}$$

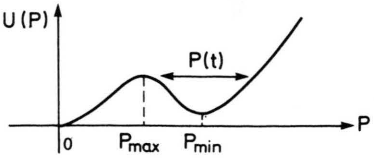

Fig. 4. Potential $U(P)$ as a function of the polarization P. The dipoles oscillate around the metastable minimum $P = P_{min}$ with $P(t) > P_{max}$ for all times.

In order to calculate the coefficients P'_{const}, A' and B' we proceed in a way, which is analogous to that applied in chapter 3.1. With the definiton

$$r'^2 = A'^2 + B'^2 \tag{24}$$

(where r' is the amplitude of the oscillation) and the formulas of the appendix we get from Eqn. (7) and Eqn. (23) a set of equations for the coefficients P'_{const}, A' and B'. It reads

$$-\omega^2 A' + K\omega B' + \omega_+^2 A' + \alpha_2 2 P'_{const} A' + \alpha_3 \frac{3}{4} r'^2 A' + \alpha_4 3 r'^2 P'_{const} A' + D \frac{5}{8} r'^4 A' = F_0 \tag{25}$$

$$-\omega^2 B' - K\omega A' + \omega_+^2 B' + \alpha_2 2 P'_{const} B' + \alpha_3 \frac{3}{4} r'^2 B' + \alpha_4 3 r'^2 P'_{const} B' + D \frac{5}{8} r'^4 B' = 0 \tag{26}$$

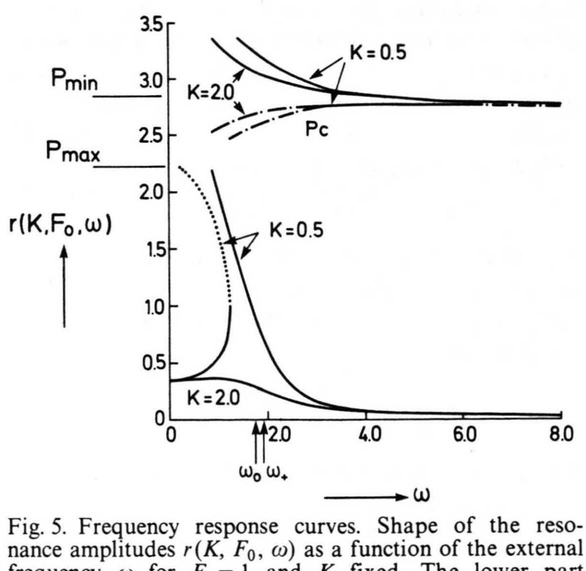

Fig. 5. Frequency response curves. Shape of the resonance amplitudes $r(K, F_0, \omega)$ as a function of the external frequency ω for $F_0 = 1$ and K fixed. The lower part belongs to the minimum $P = P_0 = 0$, the upper part to the minimum $P = P_{min}$. In the latter case, a constant shift P_c is given. Unstable branches are drawn as dashed lines, ω_0 and ω_+ are the oscillation frequencies in the limit of vanishing amplitude for the minima P_0 and P_{min}, respectively (vid. Eqns. 18 and 31).

$$\omega_+^2 P'_{const} + \alpha_2 \frac{1}{2} r'^2 + \alpha_3 \frac{3}{2} r'^2 P'_{const} + \alpha_4 \frac{3}{8} r'^4 + D \frac{15}{8} P'_{const} r'^4 = 0 \tag{27}$$

for the $\cos \omega t$, $\sin \omega t$ and constant terms, respectively. In Eqns. (25–27) the following abbreviations have been used:

$$\left.\begin{aligned} \alpha_1 &= W - 3 C P_{min}^2 + 5 D P_{min}^4 \\ \alpha_2 &= -3 C P_{min} + 10 D P_{min}^3 \\ \alpha_3 &= -C + 10 D P_{min}^2 \\ \alpha_4 &= 5 D P_{min} \end{aligned}\right\} \tag{28}$$

and

$$\omega_+^2 = W + \frac{1}{\varepsilon P^3} - 3 C P_{min}^2 + 5 D P_{min}^4 . \tag{29}$$

In the limit of a vanishing amplitude r' of the oscillation, which is determined by Eqn. (23), ω_+ would be its frequency of oscillation. From Eqn. (27) the constant term P'_{const} can be expressed as

$$P'_{const}(r) = -\frac{\alpha_2 \frac{r'^2}{2} + \alpha_4 \frac{3}{8} r'^4}{\omega_+^2 + \alpha_3 \frac{3}{2} r'^2 + D \frac{15}{8} r'^4} . \tag{30}$$

Again we can define an effective frequency $\tilde{\omega}(r')$

$$\tilde{\omega}^2(r') = \omega_+^2 + \alpha_2 2 P'_{const} + \alpha_3 \frac{3}{4} r'^2 + \alpha_4 3 P'_{const} r'^2 + D \frac{5}{8} r'^4 \tag{31}$$

with the aid of which Eqns. (25, 26) can be reduced to

$$(-\omega^2 + \tilde{\omega}^2(r')) A + K\omega B = F_0 \tag{32}$$

$$(-\omega^2 + \tilde{\omega}^2(r')) B - K\omega A = 0 . \tag{33}$$

These equations are of the same structure as Eqns. (19, 20) and are treated in an analogous way. After having calculated the resonance amplitude $r'(K, F_0, \omega)$, the constant term P'_{const} is given by Eqn. (30). The solutions $r'(\omega)$ and P'_{const} are drawn in the upper part of Fig. 5.

It is convenient to introduce a coordinate transformation

$$\left.\begin{aligned} r &= r' + P_{min} \\ P_c &= P'_{const} + P_{min} \end{aligned}\right\} \tag{34}$$

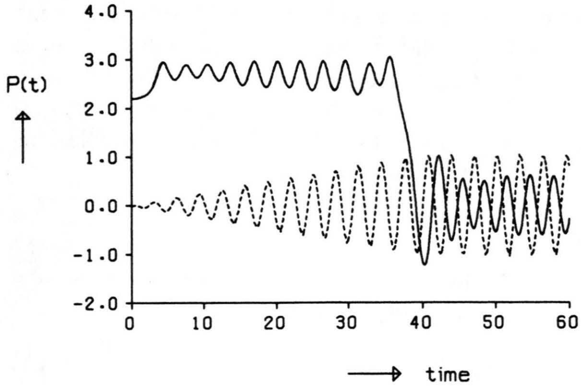

Fig. 6. Oscillation diagram. Polarization P as a function of time t. For $t = 0$ the system shows the external field, which is switched on adiabatically.

in order to discuss both resonance amplitudes, *i.e.* $P = P_0 = 0$ and $P = P_{min}$ in the same picture. The resulting resonance amplitudes are shown in the frequency response diagrams of Fig. 5.

In Fig. 6 we present the results of a numerical integration of Eqn. (7). With an increasing external field amplitude F_0 one finds a transition from the metastable state $P = P_{min}$ to a stable oscillation around the stable state $P = P_0 = 0$.

This behaviour corresponds to a transition from a highly polarized state to a nonpolarized one.

4. Shape of Absorption Lines

From an experimental point of view it would be interesting to look for the spectral properties of our model. Therefore, we take the average of the energy exchange of the system with the external field during one period of oscillation, T. This can be done by multiplying Eqn. (7) with $2\dot{P}$, followed by an integration over the period T. The result of this rather simple calculation is an equation for the energy balance system-field. It is given by

$$\underbrace{\dot{P}^2 \Big|_t^{t+T}}_{\text{kinetic energy}} + \underbrace{\omega_0^2 P^2 - \frac{c}{2} P^4 + \frac{D}{3} P^6 \Big|_t^{t+T}}_{\text{potential energy}} \tag{35}$$

$$+ \underbrace{\int_t^{t+T} 2\dot{P} K \, dt}_{\text{dissipative energy}} = \underbrace{\int_t^{t+T} 2\dot{P} F_0 \cos \omega t \, dt}_{\text{externally supplied energy}}$$

With the properties of periodicity, *i.e.*

$$\left.\begin{aligned} P(t) &= P(t+T) \\ \dot{P}(t) &= \dot{P}(t+T) \end{aligned}\right\} \tag{36}$$

Eqn. (35) can be reduced to

$$K \int_0^T \dot{P}(t)^2 \, dt = F_0 \int_0^T \dot{P}(t) \cos \omega t \, dt \,. \tag{37}$$

This equation describes the balance between the externally supplied energy and the internal losses. The energy transfer from the field to the oscillating dipoles per period T then yields

$$I(K, F_0, \omega) = \frac{1}{T} K \int_0^T \dot{P}(t)^2 \, dt \,. \tag{38}$$

The integral on the r.h.s. of Eqn. (38) can be solved in an approximative way by an application of the ansatz of Eqn. (14) and of Eqn. (23), respectively. With the definitions for the amplitudes (Eqs. (15) and (24)) we get

$$I(K, F_0, \omega) = \begin{cases} \frac{1}{2} K \omega^2 r(K, F_0, \omega)^2 \\ \frac{1}{2} K \omega^2 r'(K, F_0, \omega)^2 \end{cases} \tag{39}$$

for the minima $P = P_0$ and $P = P_{min}$. Inserting for $r(K, F_0, \omega)$ and $r'(K, F_0, \omega)$ the resonance amplitudes of our preceding calculations, we arrive at the absorption lines of the model, an example of which

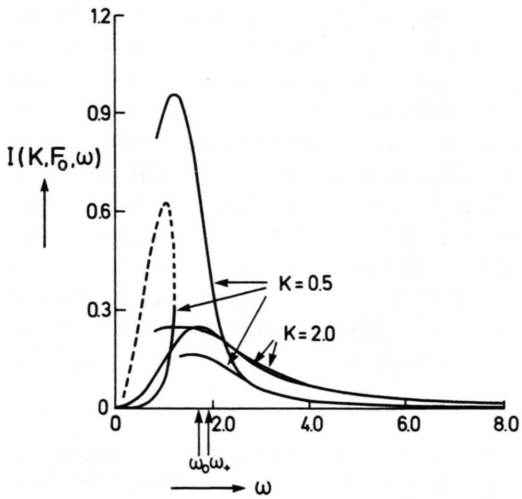

Fig. 7. Shape of absorption lines $I(K, F_0, \omega)$ as a function of the external frequency ω, calculated with the method of Harmonic Balance for the minima $P = P_0 = 0$ (curves starting at $\omega = 0$ and upper curve) and $P = P_{min}$ (other curves). The unstable branch is drawn as a dashed line, ω_0 and ω_+ are the oscillation frequencies in the limit of vanishing amplitude for P_0 and P_{min}, respectively ($F_0 = 1$).

is given in Fig. 7. The shape of the absorption lines depends on both, the strength of the external field F_0 and the magnitude of the dissipation constant K. The dependency is a nonlinear one and leads to difficulties, if one has to compare experimental findings with model predictions. Furthermore, these subtle nonlinear effects might be hidden by strong thermal effects.

5. Summary and Outlook

We have discussed the behaviour of a rather simple model, two coupled nonlinear dipole oscillators. However, one has to start with such oversimplified situations, when nonlinear dynamics are investigated.

Our model exhibits both, stable and metastable oscillations. The behaviour depends on the constant of dissipation and the external field, the latter being given by its amplitude and frequency. Small changes in these parameters can cause a switch from an oscillation around a permanently polarized state to an oscillation around a state with zero polarization in the mean and vice versa. If, for example, the internal parameters are fixed, small changes in the field amplitude F_0 can lead to drastic changes in the system's behaviour. The superposition of both, a constant and a periodic external drive yields a variety of additional transitions.

It might be desirable to deduce a microscopic basis for the model, starting from first principles. A first step towards this aim might be an expansion of our model to more than two dipoles. Furthermore, the inclusion of nonlinear dissipation might be of great relevance for externally driven nonlinear oscillators [7]. It can lead to self-excited oscillations and a competition between internal (limit cycles) and external (periodic fields) oscillations starts. A synchronisation of the system's dynamic to the external stimulus results. Furthermore, a collapse of the internal oscillation can be caused, completely triggered by external influences of extremely weak intensity, provided the system is stabilized in a highly polar state by internal means. Possible canditates for a mathematical modelling on a physical basis are biological clocks and coherent oscillations in membranes and related systems [8].

Appendix

We frequently made use of the following formulas, which easily can be derived:

$$\sin^2\alpha = \frac{1}{2}(1-\cos 2\alpha) \tag{A.1}$$

$$\cos^2\alpha = \frac{1}{2}(1+\cos 2\alpha) \tag{A.2}$$

$$\sin^3\alpha = \frac{1}{4}(3\sin\alpha - \sin 3\alpha) \tag{A.3}$$

$$\cos^3\alpha = \frac{1}{4}(3\cos\alpha + \cos 3\alpha) \tag{A.4}$$

$$\sin^4\alpha = \frac{1}{8}(\cos 4\alpha - 4\cos 2\alpha + 3) \tag{A.5}$$

$$\cos^4\alpha = \frac{1}{8}(\sin 4\alpha + 4\sin 2\alpha + 3) \tag{A.6}$$

$$\sin^5\alpha = \frac{1}{16}(\sin 5\alpha - 5\sin 3\alpha + 10\sin\alpha) \tag{A.7}$$

$$\cos^5\alpha = \frac{1}{16}(\cos 5\alpha + 5\cos 3\alpha + 10\cos\alpha)\,. \tag{A.8}$$

With these formulas the following approximated relations result:

$$(A\cos\omega t + B\sin\omega t)^2 \approx \frac{1}{2}r^2 \tag{A.9}$$

$$(A\cos\omega t + B\sin\omega t)^3 \approx \frac{3}{4}r^2(A\cos\omega t + B\sin\omega t) \tag{A.10}$$

$$(A\cos\omega t + B\sin\omega t)^4 \approx \frac{3}{8}r^4 \tag{A.11}$$

$$(A\cos\omega t + B\sin\omega t)^5 \approx \frac{5}{8}r^4(A\cos\omega t + B\sin\omega t)$$

with $r^2 = A^2 + B^2$. (A.12)

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