NONLINEAR OSCILLATIONS IN DISCRETE AND CONTINUOUS SYSTEMS

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ABSTRACT

The first thesis topic is a perturbation method for resonantly coupled nonlinear oscillators. By successive near-identity transformations of the original equations, one obtains new equations with simple structure that describe the long time evolution of the motion. This technique is related to two-timing in that secular terms are suppressed in the transformation equations. The method has some important advantages. Appropriate time scalings are generated naturally by the method, and don't need to be guessed as in two-timing. Furthermore, by continuing the procedure to higher order, one extends (formally) the time scale of valid approximation. Examples illustrate these claims. Using this method, we investigate resonance in conservative, non-conservative and time dependent problems. Each example is chosen to highlight a certain aspect of the method.

The second thesis topic concerns the coupling of nonlinear chemical oscillators. The first problem is the propogation of chemical waves of an oscillating reaction in a diffusive medium. Using two-timing, we derive a nonlinear equation that determines how spatial variations in the phase of the oscillations evolves in time. This result is the key to understanding the propogation of chemical waves. In particular, we use it to account for certain experimental observations on the Belusov-Zhabotinskii reaction.

Next, we analyse the interaction between a pair of coupled chemical oscillators. This time, we derive an equation for the phase shift, which measures how much the oscillators are out of phase. This result is the

key to understanding M. Marek's and I. Stuchl's results on coupled reactor systems. In particular, our model accounts for synchronization and its bifurcation into rhythm splitting.

Finally, we analyse large systems of coupled chemical oscillators. Using a continuum approximation, we demonstrate mechanisms that cause auto-synchronization in such systems.

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INTRODUCTION

In Part I, we develop a perturbation method for resonantly coupled nonlinear oscillators. By performing successive near identity transformations of the original equations, one obtains new equations with simple structure that describe the long time evolution of the motion. The technique is related to two-timing in that secular terms are suppressed in the transformation equations. There are some important advantages. Appropriate time scalings are generated naturally by the method, and don't have to be guessed as in two timing. Furthermore, by continuing the procedure to higher order, one extends (formally) the time scale of validity. This is in marked contrast to two timing, where continuation to higher order only improves the accuracy in the same fixed time interval.

The idea of a perturbation method based on transformations of the dependent variables is already known in certain limited contexts. Von Zeipels procedure [1] treats Hamiltonian systems via successive canonical transformations. Elimination of secular terms in the transformations determines the form of the Hamiltonian in the new variables. The details of Von Zeipel's procedure depend on the Hamiltonian structure of the equations that it treats. But the basic idea of performing near identity transformations and suppressing secular terms in the transformation equations is much more general. The generalizations of Von Zeipel's method to non-conservative, time dependent problems is one of the main topics of this study.

In Chapter 1, we treat a special case of the three-body problem. Aside from its intrinsic interest, we include this example as an exercise

of Von Zeipel's method on a problem whose zero order description is nonlinear. In Chapter 2, we draw on the experience with Von Zeipel's method to develop a method of near-identity transformations for non-conservative systems. Specifically, we treat the resonant coupling of two Van der Pol oscillators. In Chapter 3, we study the application of the near identity transformation method to time dependent problems. Specifically, we treat the passage through resonance of a forced oscillator with slowly varying frequency. In this example, we see how the near identity transformation method determines the characteristic time scales in a resonant system. Finally, Chapter 4 is a demonstration of how the time scale of valid approximation is extended by carrying out the near-identity procedure to higher order. We study the mechanism by which the motion of an autonomous system approaches a limit cycle on one time scale and then evolves away from this initial limit cycle on a longer time scale. This contrasts itself with the usual behavior of limit cycle oscillations, where the motion evolves to a stable periodic solution whose amplitude and frequency are fixed for all time.

In Part II, we study nonlinear chemical oscillations in certain continuous and discrete systems. In Chapter 5, we analyze a model of an oscillating chemical reaction taking place in a diffusive medium. Using a two timing method, we derive a nonlinear equation that determines how the spatial variations in the phase of the oscillations evolves in time. This result is the key to understanding the propagation of chemical waves, In particular, we use it to account forcertain experimental observations on the Bekysiv-Zhabotinskii reaction.

In Chapter 6, we study the interaction between a pair of coupled

chemical oscillators. Using a two-timing procedure similar to the one employed in Chapter 5, we derive an equation that governs the time evolution of the phase shift, which measures how much the oscillators are out of phase. This result is used to interpret experimental observations on coupled reactor systems. In particular, our model accounts for synchronization, and its bifurcation into rhythm splitting.

In Chapter 7, we study the mechanisms that underlie synchronization processes in large systems of coupled chemical oscillators. Specifically, we study the evolution from an initial state where the phases of the oscillators are distributed randomly, to a final state where all the oscillators are in phase. In the continuum limit, where there are many oscillators per unit volume, we derive a nonlinear integro-differential equation that describes how the distribution of the oscillator's phases evolves in time. In general, this problem is very formidable. But we discover some important special cases for which there are exact solutions describing synchronization processes.

Part I

THE METHOD OF NEAR IDENTITY TRANSFORMATIONS

CHAPTER 1

RESONANCE IN A PLANETARY ORBIT

We study the evolution of a resonantly perturbed planetary orbit. In polar variables r, ϕ, the Hamiltonian is

$$H = \tfrac{1}{2}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right) - \frac{1}{r} + \varepsilon r \cos(\phi - \varepsilon\omega t) \quad , \tag{1}$$

where p_r and p_ϕ are the momenta conjugate to r and ϕ, and $\varepsilon << 1$. The perturbation term $\varepsilon\, r \cos(\phi - \varepsilon\omega t)$ can be thought of as the influence of a second, much more distant planet with a long period. Using Von Zeipel's transformation procedure, we will show how this perturbation leads to an internal resonance between the degrees of freedom. The resonance manifests itself by large amplitude, long period oscillations in the angular momentum of the orbit. The effect is clearly visible in Figure 1.2, which depicts a typical trajectory obtained from a numerical simulation.

We adopt a coordinate system that rotates with the perturbing field. Under the transformation $R = r$, $\Phi = \phi - \varepsilon\omega t$, the Hamiltonian becomes

$$H = H^0 + \varepsilon\, H^1 \quad , \tag{2}$$

where

$$H^0 \equiv \tfrac{1}{2}\left(p_R^2 + \frac{p_\Phi^2}{R^2}\right) - \frac{1}{R} \tag{3}$$

and

$$H^1 \equiv R \cos \Phi - \omega p_\Phi \quad . \tag{4}$$

In this coordinate system, the Hamiltonian is time independent.

It is convenient to introduce the action angle variables $(\alpha_R, \alpha_\Phi, \nu_R, \nu_\Phi)$ of the unperturbed Hamiltonian H^o [2]. The transformation from polar variables (p_R, p_Φ, R, Φ) to action angle variables is given implicitly by

$$\alpha_R = - p_\Phi + \frac{1}{\sqrt{-2H^o}} \quad , \tag{5}$$

$$\alpha_\Phi = p_\Phi \quad , \tag{6}$$

$$R = a(1 - e \cos \zeta) \quad , \tag{7}$$

$$\Phi = \nu_\Phi - \nu_R + \arccos \left\{ \frac{\cos \zeta - e}{1 - e \cos \zeta} \right\} \quad , \tag{8}$$

where

$$a \equiv - \frac{1}{2H^o} \quad \text{and} \quad e = \{1 + 2H^o \alpha_\Phi^2\}^{\frac{1}{2}} \tag{9}$$

and $\zeta = \zeta(\nu_R)$ is determined from

$$\nu_R = \zeta - e \sin \zeta \quad . \tag{10}$$

In action angle variables, the unperturbed Hamiltonian H^o is

$$H^o = -\frac{1}{2(\alpha_R + \alpha_\Phi)^2} \quad , \tag{11}$$

and the perturbation term $H^1 = R\cos\Phi - \omega p_\Phi$ can be written as

$$H^1 = a\cos\psi(\cos\zeta - e) - a\sqrt{1-e^2}\sin\psi\sin\zeta - \omega\alpha_\Phi \tag{12}$$

where

$$\psi \equiv \nu_\Phi - \nu_R \quad . \tag{13}$$

The actions α_R and α_Φ are constants of the unperturbed ($\varepsilon = 0$) motion. In particular, α_Φ is the angular momentum. a and e are the major axis and eccentricity of an unperturbed orbit. The angles ν_R and ν_Φ have $\dot{\nu}_R = \dot{\nu}_\Phi = \frac{1}{(\alpha_R + \alpha_\Phi)^3}$ for the unperturbed motion, in which case $\psi = \nu_\Phi - \nu_R$ is another constant. Physically, ψ is the angle along which the major axis of the orbit is aligned.

When $\varepsilon \neq 0$, α_R, α_Φ and ψ are no longer constants of the motion, but vary slowly in time. Our aim is to find an asymptotic solution which describes the slow evolution of α_R, α_Φ and ψ. Following Von Zeipel's method, we construct a near identity canonical transformation $(\underset{\sim}{\alpha}, \underset{\sim}{\nu}) \equiv (\alpha_R, \alpha_\Phi, \nu_R, \nu_\Phi) \to (\underset{\sim}{A}, \underset{\sim}{\Theta}) \equiv (A_R, A_\Phi, \Theta_R, \Theta_\Phi)$ so that the equations of motion for $(\underset{\sim}{A}, \underset{\sim}{\Theta})$ are integrable.

The canonical transformation can be expressed in terms of a generating function $S(\underset{\sim}{A}, \underset{\sim}{\nu}, \varepsilon)$ via

$$\underset{\sim}{\alpha} = \nabla_{\underset{\sim}{\nu}} S \ , \ \underset{\sim}{\theta} = \nabla_{\underset{\sim}{A}} S \ . \tag{14}$$

Under the action of the transformation $(\underset{\sim}{\alpha}, \underset{\sim}{\nu}) \to (\underset{\sim}{A}, \underset{\sim}{\theta})$, the Hamiltonian assumes a new form $E(\underset{\sim}{A}, \underset{\sim}{\theta}, \varepsilon)$. That is,

$$H(\underset{\sim}{\alpha}, \underset{\sim}{\nu}, \varepsilon) = H^{o}(\underset{\sim}{\alpha}) + \varepsilon H^{1}(\underset{\sim}{\alpha}, \underset{\sim}{\nu}) = E(\underset{\sim}{A}, \underset{\sim}{\theta}, \varepsilon) \ . \tag{15}$$

Combining (14) and (15), we find

$$H^{o}(\nabla_{\underset{\sim}{\nu}} S) + \varepsilon H^{1}(\nabla_{\underset{\sim}{\nu}} S, \underset{\sim}{\nu}) = E(\underset{\sim}{A}, \nabla_{\underset{\sim}{A}} S) \ . \tag{16}$$

This is the Hamilton-Jacobi equation. It is a relationship between the generating function $S(\underset{\sim}{A}, \underset{\sim}{\nu}, \varepsilon)$ and the new form of the Hamiltonian $E(\underset{\sim}{A}, \underset{\sim}{\theta}, \varepsilon)$.

When $\varepsilon = 0$, the equations of motion are integrable in the $(\underset{\sim}{\alpha}, \underset{\sim}{\nu})$ variables, and the transformation (14) should reduce to the identity. Hence, we assume that $S(\underset{\sim}{A}, \underset{\sim}{\nu}, \varepsilon)$ and $E(\underset{\sim}{A}, \underset{\sim}{\theta}, \varepsilon)$ have the asymptotic forms

$$S \sim \underset{\sim}{A} \cdot \underset{\sim}{\nu} + \varepsilon S^{1}(\underset{\sim}{A}, \underset{\sim}{\nu}) + O(\varepsilon^{2}) \ , \tag{17}$$

$$E \sim H^{o}(\underset{\sim}{A}) + \varepsilon E^{1}(\underset{\sim}{A}, \underset{\sim}{\theta}) + O(\varepsilon^{2}) \tag{18}$$

as $\varepsilon \to 0$. Substituting (17) and (18) into the Hamiltonian-Jacobi equation (16), we find

$$\nabla_{\underset{\sim}{\alpha}} H^o(A) \cdot \nabla_{\underset{\sim}{\nu}} S^1 = E^1(\underset{\sim}{A}, \underset{\sim}{\nu}) - H^1(\underset{\sim}{A}, \underset{\sim}{\nu}) \quad . \tag{19}$$

Using the specific forms of H^o and H^1 given in (11) and (12), this becomes

$$\frac{1}{a^3} LS^1 = E^1(\underset{\sim}{A}, \underset{\sim}{\nu}) - a \cos\psi(\cos\zeta - e) - a\sqrt{1-e^2}\sin\psi\sin\zeta - \omega A_\Phi . \tag{20}$$

where a and e are evaluated at $\underset{\sim}{\alpha} = \underset{\sim}{A}$, and $LS^1 \equiv \frac{\partial S^1}{\partial \nu_R} + \frac{\partial S^1}{\partial \nu_\Phi}$ is the directional derivative of S^1 along lines $\psi = \nu_\Phi - \nu_R = \text{constant}$.

We require a solution for S^1 that is bounded in the angles ν_R and ν_Φ, so that the transformation $(\underset{\sim}{\alpha}, \underset{\sim}{\nu}) \to (\underset{\sim}{A}, \underset{\sim}{\Theta})$ defined in (14) remains uniformly near the identity as ν_R, ν_Φ become infinite. Hence E^1 must be chosen so that the right hand side of (20) has no non-zero component that is constant along the lines $\psi = \nu_\Phi - \nu_R = \text{constant}$. Otherwise, S^1 will have secular terms proportional to ν_R and ν_Φ. The simplest choice for E^1 that does the job is

$$E^1 = a\cos\psi\,\frac{1}{2\pi}\int_0^{2\pi}(\cos\zeta(\nu_R) - e)d\nu_R + a\sqrt{1-e^2}\sin\psi\,\frac{1}{2\pi}\int_0^{2\pi}\sin\zeta(\nu_R)d\nu_R + \omega A_\Phi \quad . \tag{21}$$

Here, we recall that ζ is a function of ν_R, defined implicitly by (10). Using the definition (10) of $\zeta(\nu_R)$, we compute

$$\int_0^{2\pi} \cos\,\zeta(\nu_R)d\nu_R = \int_0^{2\pi} \cos\,\zeta\,\frac{d\nu_R}{d\zeta}\,d\zeta =$$

$$\int_0^{2\pi} \cos\,\zeta(1 - e\,\cos\,\zeta)d\zeta \;= -\,\pi\,e \quad . \tag{22}$$

Similarly, we find

$$\int_0^{2\pi} \sin\,\zeta(\nu_R)d\nu_R = 0 \quad . \tag{23}$$

Hence, (21) reduces to

$$E^1(\underset{\sim}{A},\ \underset{\sim}{\nu}) = U(\underset{\sim}{A},\ \psi) \equiv -\,\frac{3}{2}\,ae\,\cos\,\psi + \omega A_\Phi \quad . \tag{24}$$

With this choice of E^1, (20) can be integrated to find a bounded solution for S^1.

In $(\underset{\sim}{A},\ \underset{\sim}{\Theta})$ coordinates, the Hamiltonian is

$$E(\underset{\sim}{A},\ \underset{\sim}{\Theta},\ \varepsilon) = H^o(\underset{\sim}{A}) + \varepsilon\ U(\underset{\sim}{A},\ \Psi) + o(\varepsilon^2) \quad , \tag{25}$$

where

$$\Psi \equiv \Theta_\Phi - \Theta_R \quad . \tag{26}$$

Hence, for times $t < O(\frac{1}{\varepsilon^2})$, the motion is described to $O(1)$ accuracy by

$$\dot{A}_R = -\frac{\partial E}{\partial \Theta_R} = \varepsilon \frac{\partial U}{\partial \Psi} \quad , \tag{27}$$

$$\dot{A}_\Phi = -\frac{\partial E}{\partial \Theta_\Phi} = -\varepsilon \frac{\partial U}{\partial \Psi} \quad , \tag{28}$$

$$\dot{\Theta}_R = \frac{\partial E}{\partial A_R} = \frac{\partial H^0}{\partial A_R} + \varepsilon \frac{\partial U}{\partial A_R} \quad , \tag{29}$$

$$\dot{\Theta}_\Phi = \frac{\partial E}{\partial A_\Phi} = \frac{\partial H^0}{\partial A_\Phi} + \varepsilon \frac{\partial U}{\partial A_\Phi} \quad . \tag{30}$$

This system is completely integrable. From (27) and (28), we see that

$$A \equiv A_R + A_\Phi \tag{31}$$

is a constant of the motion. The equations (29) and (30) for Θ_R and Θ_Φ can be subtracted from each other to yield a single equation for Ψ in terms of $\underset{\sim}{A}$ and Ψ. One finds

$$\dot{\Psi} = \Theta_\Phi - \Theta_R = \varepsilon\left(\frac{\partial U}{\partial A_\Phi} - \frac{\partial U}{\partial A_R}\right) \quad . \tag{32}$$

Here, we have used the fact that $\frac{\partial H^0}{\partial A_R}$ and $\frac{\partial H^0}{\partial A_\Phi}$ are both equal to $\frac{1}{(A_R+A_\Phi)^3}$. Hence, these terms cancel each other out in the subtraction, and don't appear in (32). From these preceding observations, we see that the fourth order system (27) - (30) can be reduced to a second order system for the angular momentum A_Φ and the angle of orientation Ψ of the orbits' major axis. We find

$$\dot{A}_\Phi = - \varepsilon \frac{\partial U}{\partial \Psi} (A-A_\Phi, A_\Phi, \Psi) \quad , \tag{33}$$

$$\dot{\Psi} = \varepsilon \frac{\partial U}{\partial A_\Phi} (A-A_\Phi, A_\Phi, \Psi) - \varepsilon \frac{\partial U}{\partial A_R} (A-A_\Phi, A_\Phi, \Psi) \quad . \tag{34}$$

It is easily verified that this is a second order Hamiltonian system, with Hamiltonian $U(A-A_\Phi, A_\Phi, \Psi)$. The level lines of $U(A-A_\Phi, A_\Phi, \Psi)$ give the trajectories of the A_Φ, Ψ phase plane. Once these are known, the solution of (33) and (34) is reduced to direct quadrature.

We study in detail the evolution of the angular momentum A_Φ. From the definition (24) of U, and the definitions (9) of a and e, one finds

$$U(A - A_\Phi, A_\Phi, \Psi) = - \frac{3}{2} a\, e \cos \Psi + \omega A_\Phi =$$

$$- \frac{3}{2} A\sqrt{A^2-A_\Phi^2} \cos \Psi + \omega A_\Phi \quad . \tag{35}$$

Hence, the equation (33) for the angular momentum reads

$$\frac{dA_\Phi}{d\tau} = \frac{3}{2} A\sqrt{A^2-A_\Phi^2} \sin \Psi \quad , \tag{36}$$

where τ is the slow time εt. Squaring (36) gives

$$\left(\frac{dA_\Phi}{d\tau}\right)^2 = \frac{9}{4} A^2(A^2-A_\Phi^2) - \frac{9}{4} A^2(A^2 - A_\Phi^2) \cos^2 \Psi \quad . \tag{37}$$

With the help of (35), the second term in the right hand side of (37) can be written as $(U - \omega A_\Phi)^2$. Hence, (37) becomes

$$\left(\frac{dA_\Phi}{d\tau}\right)^2 = \frac{9}{4} A^2(A^2 - A_\Phi^2) - (U - \omega A_\Phi)^2 \quad . \tag{38}$$

Differentiating (38) with respect to τ once gives

$$\frac{d^2A_\Phi}{d\tau^2} + (\frac{9}{4} A^2 + \omega^2)A_\Phi = - 2 U \omega \quad . \tag{39}$$

From this equation, we see immediately that the angular momentum oscillates sinusoidally about the mean value $- \frac{2U\omega}{\frac{9}{4}A^2\omega^2}$ with period

$$\tau_0 = \frac{2\pi}{\sqrt{\frac{9}{4} A^2 + \omega^2}} \tag{40}$$

in the slow time $\tau = \varepsilon t$. The amplitude ρ of the oscillations can be determined from the zeros of

$$\left(\frac{dA_\Phi}{d\tau}\right)^2 = \frac{9}{4} A^2(A^2 - A_\Phi^2) - (U - \omega A_\Phi)^2 = 0 \quad . \tag{41}$$

For orbits that are circular at some point in their evolution there is a time when the eccentricity $e = \left\{1 - \frac{A_\Phi^2}{A^2}\right\}^{1/2}$ is zero. At that time,

$A_\Phi = A$. Substituting $A_\Phi = A$ into (35) gives $U = \omega A$. With this value of U, we find from (42) that

$$\rho = A \left\{\frac{1}{1 + (\frac{2}{3}\frac{\omega}{A})^2}\right\} \quad . \tag{42}$$

Figure 1.1 shows a graph of ρ vs. ω. We see that the resonance is strongest when $\omega = 0$ and weakens as $\omega \to \pm \infty$. This result is easy to understand physically. As ω increases, the perturbing field in (1) rotates more rapidly. If the perturbing field undergoes many oscillations during the period of the planet's orbit, its cumulative effect on the orbit will be small.

We compare the results of the theory with a numerical simulation. Figure 1.2 shows the numerically computed evolution of an initially circular orbit of radius $\frac{1}{2}$ for the case $\varepsilon = .05$, $\omega = 1.4$. Figure 1.3 is the corresponding plot of the angular momentum. From this plot, we estimate the amplitude and period of the oscillations in the angular momentum, and compare them with theoretical values given by (39) and (42). The results are shown in the table below.

	$T_0 \equiv \frac{\tau_0}{\varepsilon}$	ρ
Numerical value	~ 71	~ .251
Theory value	71.55	.258

CHAPTER 2

RESONANT INTERACTION OF COUPLED VAN DER POL OSCILLATORS

We develop a near identity transformation procedure that treats internal resonance in systems of non-conservative oscillators. For a concrete model problem, we analyze the interaction between two coupled Van der Pol oscillators. The equations of motion are

$$\begin{aligned} \ddot{u}_1 + \varepsilon\dot{u}_1(u_1^2 - 1) + u_1 &= \varepsilon\dot{u}_2 \quad , \\ \ddot{u}_2 + \varepsilon\dot{u}_2(u_2^2 - 1) + (1 + 2\varepsilon\omega)u_2 &= \varepsilon\dot{u}_1 \quad , \end{aligned} \tag{1}$$

where ω is a constant, and $0 < \varepsilon << 1$. When $\omega = 0$, two identical oscillators are coupled. When $\omega \neq 0$, two different oscillators are coupled.

It is convenient to write (1) as a system of first order equations. Setting $v_k = \dot{u}_k$, $k = 1,2$, (1) can be recast as

$$\begin{aligned} \dot{u}_1 &= v_1 \quad , \\ \dot{v}_1 &= -u_1 - \varepsilon\{v_1(u_1^2 - 1) - v_2\} \quad , \\ \dot{u}_2 &= v_2 \quad , \\ \dot{v}_2 &= -u_2 - \varepsilon\{v_2(u_2^2 - 1) + 2\omega u_2 - v_1\} \quad . \end{aligned} \tag{2}$$

The solutions for $\varepsilon = 0$ are

$$u_k = r_k \cos(t + \beta_k) \quad , \quad v_k = -r_k \sin(t + \beta_k) \quad , \quad k = 1,2, \tag{3}$$

where r_k and β_k are constants. This suggests a change of dependent variables $(u_k, v_k) \to (r_k, \nu_k)$ given by

$$u_k = r_k \cos \nu_k \ , \ v_k = - r_k \sin \nu_k \ , \ k = 1,2 \ . \tag{4}$$

The equations for the amplitudes r_k and phases ν_k are

$$\begin{aligned}
\dot{r}_1 &= \varepsilon\{f(r_1, \nu_1) + \varphi(r_1, r_2, \nu_1, \nu_2)\} \ , \\
\dot{r}_2 &= \varepsilon\{f(r_2, \nu_2) + \varphi(r_2, r_1, \nu_2, \nu_1) + \omega\, r_2 \sin 2\nu_2\} \ , \\
\dot{\nu}_1 &= 1 + \varepsilon\{g(r_1, \nu_1) + \gamma(r_1, r_2, \nu_1, \nu_2)\} \ , \\
\dot{\nu}_2 &= 1 + \varepsilon\{g(r_2, \nu_2) + \gamma(r_2, r_1, \nu_2, \nu_1) + \omega(1 + \cos 2\nu_2)\} \ ,
\end{aligned} \tag{5}$$

where

$$f(r, \nu) \equiv r \sin^2 \nu\{1 - r^2 \cos^2 \nu\} = \frac{r}{2}\left(1 - \frac{r^2}{4}\right) - \frac{r}{2} \cos 2\nu + \frac{r^3}{8} \cos 4\nu \ , \tag{6}$$

$$g(r, \nu) \equiv \sin \nu \cos \nu\{1 - r^2 \cos^2 \nu\} = \tfrac{1}{2}\left(1 - \frac{r^2}{2}\right) \sin 2\nu - \frac{r^2}{8} \sin 4\nu \ , \tag{7}$$

$$\varphi(r_1, r_2, \nu_1, \nu_2) \equiv r_2 \sin \nu_1 \sin \nu_2 = \frac{r_2}{2}\{\cos(\nu_2 - \nu_1) - \cos(\nu_1 + \nu_2)\} \ , \tag{8}$$

$$\gamma(r_1, r_2, \nu_1, \nu_2) \equiv \frac{r_2}{r_1} \cos \nu_1 \cos \nu_2 = \tfrac{1}{2} \frac{r_2}{r_1}\{\sin(\nu_2 - \nu_1) + \sin(\nu_1 + \nu_2)\} \tag{9}$$

When $\varepsilon = 0$, the equations (5) reduce to

$$\dot{r}_1 = \dot{r}_2 = 0 \text{ and } \dot{\nu}_1 = \dot{\nu}_2 = 1 \ . \tag{10}$$

Hence, r_1, r_2 and $\psi \equiv \nu_2 - \nu_1$ are constants of the motion for $\varepsilon = 0$. When $\varepsilon \neq 0$, r_1, r_2 and ψ are no longer constants, but vary slowly in time. To find an asymptotic solution of (5) that describes the slow evolution of r_1, r_2 and ψ, we introduce a near identity transformation $(\underset{\sim}{r}, \underset{\sim}{\nu}) \to (\underset{\sim}{R}, \underset{\sim}{\Theta})$. We assume that this transformation has the asymptotic form

$$\begin{aligned} r_k &= R_k + \varepsilon\, S_k(\underset{\sim}{R}, \underset{\sim}{\Theta}) + 0(\varepsilon^2) \quad , \\ \nu_k &= \Theta_k + \varepsilon\, T_k(\underset{\sim}{R}, \underset{\sim}{\Theta}) + 0(\varepsilon^2) \quad , \end{aligned} \tag{11}$$

and the equations of motion in the new variables are

$$\begin{aligned} \dot{R}_k &= \varepsilon\, F_k(\underset{\sim}{R}, \underset{\sim}{\Theta}) + 0(\varepsilon^2) \quad , \\ \dot{\Theta}_k &= 1 + \varepsilon\, G_k(\underset{\sim}{R}, \underset{\sim}{\Theta}) + 0(\varepsilon^2) \quad . \end{aligned} \tag{12}$$

Substituting (11) into the system (5) and comparing the result with (12), we see that

$$LS_1 = f(R_1, \Theta_1) + \varphi(R_1, R_2, \Theta_1, \Theta_2) - F_1(\underset{\sim}{R}, \underset{\sim}{\Theta}) \quad , \tag{13}$$

$$LS_2 = f(R_2, \Theta_2) + \varphi(R_2, R_1, \Theta_2, \Theta_1) + \omega R_2 \sin 2\Theta_2 - F_2(\underset{\sim}{R}, \underset{\sim}{\Theta}), \tag{14}$$

$$LT_1 = g(R_1, \Theta_1) + \gamma(R_1, R_2, \Theta_1, \Theta_2) - G_1(\underset{\sim}{R}, \underset{\sim}{\Theta}) \quad , \tag{15}$$

$$LT_2 = g(R_2, \Theta_2) + \gamma(R_2, R_1, \Theta_2, \Theta_1) + \omega(1 + \cos 2\Theta_2) - G_2(\underset{\sim}{R}, \underset{\sim}{\Theta}) \quad , \tag{16}$$

where $L \equiv \dfrac{\partial}{\partial \Theta_1} + \dfrac{\partial}{\partial \Theta_2}$ is the directional derivative along the lines

$\Psi \equiv \Theta_2 - \Theta_1$ = constant of the (Θ_1, Θ_2) plane.

We require solutions for the S_k and T_k that are bounded as the phases Θ_1, Θ_2 become infinite, so that the transformation $(\underset{\sim}{r}, \underset{\sim}{\nu}) \to (\underset{\sim}{R}, \underset{\sim}{\Theta})$ defined by (11) is uniformly near the identity for all Θ_1 and Θ_2. This boundedness requirement leads to natural choices for the F_k and G_k. Consider, as an example, the equation (13) for S_1. Since LS^1 is the directional derivative of S^1 along lines $\Psi = \Theta_2 - \Theta_1$ = constant, we must choose F_1 to suppress any non-zero component of $f(R_1, \Theta_1)$ or $\varphi(R_1, R_2, \Theta_1, \Theta_2)$ which is constant along the lines $\Psi = \Theta_2 - \Theta_1$ = constant. Otherwise S^1 will have secular terms proportional to Θ_1 and Θ_2. From the definitions (6) and (8) of f and φ, we see that it is sufficient to take

$$F_1 = \frac{R_1}{2}\left(1 - \frac{R_1^2}{2}\right) + \frac{R_2}{2}\cos\Psi \quad . \tag{17}$$

Similarly, we choose

$$F_2 = \frac{R_2}{2}\left(1 - \frac{R_2^2}{4}\right) + \frac{R_1}{2}\cos\Psi \quad , \tag{18}$$

$$G_1 = \tfrac{1}{2}\frac{R_2}{R_1}\sin\Psi \quad , \tag{19}$$

$$G_2 = \omega - \tfrac{1}{2}\frac{R_1}{R_2}\sin\Psi \quad . \tag{20}$$

With these choices for the F_k and G_k, (13) - (16) can be integrated to find bounded values for the S_k and T_k.

In $(\underset{\sim}{R}, \underset{\sim}{\Theta})$ variables, the equations of motion are

$$
\begin{aligned}
\dot{R}_1 &= \varepsilon \frac{R_1}{2}\left(1 - \frac{R_1^2}{4}\right) + \varepsilon \frac{R_2}{2}\cos\Psi + 0(\varepsilon^2) \quad , \\
\dot{R}_2 &= \varepsilon \frac{R_2}{2}\left(1 - \frac{R_2^2}{4}\right) + \varepsilon \frac{R_1}{2}\cos\Psi + 0(\varepsilon^2) \quad , \\
\dot{\Theta}_1 &= 1 + \varepsilon \tfrac{1}{2}\frac{R_2}{R_1}\sin\Psi + 0(\varepsilon^2) \quad , \\
\dot{\Theta}_2 &= 1 + \varepsilon\omega - \varepsilon \tfrac{1}{2}\frac{R_1}{R_2}\sin\psi + 0(\epsilon^2) \quad ,
\end{aligned}
\tag{21}
$$

where $\Psi \equiv \Theta_2 - \Theta_1$. These can be reduced to a third order system by subtracting the equations for Θ_1 and Θ_2 to form a single equation for Ψ. The system for R_1, R_2 and Ψ can be written as

$$
\begin{aligned}
\frac{dR_1}{d\tau} &= \frac{R_1}{2}\left(1 - \frac{R_1^2}{4}\right) + \frac{R_2}{2}\cos\Psi + 0(\varepsilon) \quad , \\
\frac{dR_2}{d\tau} &= \frac{R_2}{2}\left(1 - \frac{R_2^2}{4}\right) + \frac{R_1}{2}\cos\Psi + 0(\varepsilon) \quad , \\
\frac{d\Psi}{d\tau} &= \omega - \frac{R_1^2 + R_2^2}{2R_1R_2}\sin\Psi + 0(\varepsilon) \quad ,
\end{aligned}
\tag{22}
$$

where τ is the slow time εt.

When $|\omega| < 1$, (22) has a stable steady state solution with $R_1 = R_2 = R_0$ and $\Psi = \Psi_0$, where Ψ_0 is the solution of

$$
\omega = \sin\Psi_0 \tag{23}
$$

with $-\frac{\pi}{2} < \Psi_0 < \frac{\pi}{2}$, and

$$R_0 = 2\{1 + (1 - \omega^2)^{\frac{1}{2}}\}^{\frac{1}{2}} \quad . \tag{24}$$

These correspond to synchronized states, where the phase difference $\Psi(\tau)$ is a constant. Notice that R_0 is greater than 2, which is the amplitude of an unperturbed Van der Pol oscillator.

When ω is increased to a value greater than one, this stable steady state is lost. Instead, one finds a solution with R_1 and R_2 both equal to the same periodic function $R(\tau)$. In the case $R_1 = R_2 = R$, (22) reduces to

$$\frac{dR}{d\tau} = \frac{R}{2}(1 + \cos \Psi) - \frac{R^3}{8} \quad , \tag{25}$$

$$\frac{d\Psi}{d\tau} = \omega - \sin \Psi \quad . \tag{26}$$

The equation for the phase difference Ψ is decoupled from the amplitude R, and can be solved seperately. We consider the limiting case where ω is slightly greater than one, so that $0 < \omega - 1 << 1$. Figure 2.1 illustrates the situation with a graph of $\frac{d\Psi}{d\tau}$ vs. Ψ. The solution for Ψ is nearly constant at the values $\Psi = \frac{\pi}{2} + 2\pi\, m$, m = integer, where $\frac{d\Psi}{d\tau} = \omega - \sin \Psi$ is $o(1)$. Away from $\Psi = \frac{\pi}{2} + 2\pi\, m$, $\frac{d\Psi}{d\tau}$ is $O(1)$. These regions of rapid variations in $\Psi(\tau)$ correspond to boundary layers that join the constant values $\Psi = \frac{\pi}{2} + 2\pi\, m$, as shown in Figure 2.2. The interval of τ between two successive boundary layers is

$$\tau_0 = \int_0^{2\pi} \frac{d\Psi}{\omega - \sin \Psi} = \frac{4\pi}{\sqrt{\omega^2 - 1}} \quad . \tag{27}$$

In the boundary layer regions, Ψ has the analytical form

$$\Psi = 2 \arctan \tau - \frac{\pi}{2} + 2\pi m + O(\omega-1) \quad . \tag{28}$$

Once Ψ is known, R can be computed from (25). Equation (25) can be converted into a linear ODE by introducing the change of variable $S = \frac{1}{R^2}$. The equation for S is

$$\frac{dS}{d\tau} = - (1 + \cos \Psi) S + \tfrac{1}{4} \quad . \tag{29}$$

One solution is

$$S = \tfrac{1}{4} \int_0^\infty e^{-y} \, e^{\int_\tau^{\tau-y} \cos \Psi(\zeta) d\zeta} \, dy \quad . \tag{30}$$

Since $\Psi(\zeta)$ increases by 2π when ζ increases by 2π, it follows that $\cos \Psi(\zeta)$ is 2π periodic in ζ. Hence, (30) is the periodic solution of (29). There is a useful alternative form of (30). Differentiating (26) with respect to τ gives

$$\frac{d^2\Psi}{d\tau^2} = - \cos \Psi \frac{d\Psi}{d\tau} \quad . \tag{31}$$

Hence,

$$\int_\tau^{\tau-y} \cos \Psi(\zeta) d\zeta = - \log \left\{ \frac{\frac{d\Psi}{d\tau} (\tau-y)}{\frac{d\Psi}{d\tau} (\tau)} \right\} \quad , \tag{32}$$

and (30) becomes

$$S = \tfrac{1}{4} \frac{d\Psi}{d\tau} \int_0^\infty \frac{e^{-y}}{\frac{d\Psi}{d\tau}(\tau-y)}\, dy \quad . \tag{33}$$

To find the behavior of S in the boundary layer regions, we substitute into (33) the approximate form of Ψ given in (28). We find

$$S \sim \tfrac{1}{4} \frac{1}{1+\tau^2} \int_0^\infty e^{-y}\{1 + (\tau-y)^2\}dy = \tfrac{1}{4} \frac{2+(\tau-1)^2}{1+\tau^2} \quad . \tag{34}$$

The corresponding value of $R(\tau) = \dfrac{1}{\sqrt{S(\tau)}}$ is

$$R(\tau) = \frac{2\sqrt{1+\tau^2}}{\sqrt{2 + (\tau-1)^2}} \quad . \tag{35}$$

Figure 2.3 is a plot of this inner solution for R. Notice that $R(\tau)\to 2$ as $|\tau| \to \infty$. At each τ where a boundary layer in Ψ occurs, $R(\tau)$ undergoes the oscillation depicted in Figure 2.3. Figure 2.4 depicts the solution for $R(\tau)$. We see that long intervals in which $R(\tau)$ is nearly constant are punctuated by brief intervals where $R(\tau)$ undergoes an oscillation.

CHAPTER 3

PASSAGE THROUGH RESONANCE

For a time dependent problem, we examine the passage through resonance of a forced oscillator with slowly varying frequency. The equation of motion is

$$\ddot{x} + \omega^2(\varepsilon t)x = \varepsilon\, a \cos t \quad , \tag{1}$$

where $0 < \varepsilon << 1$. (1) can be recast as a pair of first order equations for the amplitude and phase of the oscillations. The amplitude r and phase ν are related to x by $x = r \cos \nu$. The equations for r and ν are

$$\dot{r} = \varepsilon f(r, \nu, t) \ , \ \dot{\nu} = \omega + \varepsilon g(r, \nu, t) \quad , \tag{2}$$

where

$$f \equiv -\frac{r\omega'}{2\omega} + \frac{r\omega'}{2\omega} \cos 2\nu + \frac{a}{2\omega} \sin(t-\nu) - \frac{a}{2\omega} \sin(t+\nu) \tag{3}$$

and

$$g \equiv -\frac{\omega'}{2\omega} \sin 2\nu - \frac{a}{2\omega r} \cos(t-\nu) - \frac{a}{2\omega r} \cos(t+\nu) \quad . \tag{4}$$

To find the asymptotic solution of (2), we introduce a near identity transformation $(r,\nu) \to (R,\theta)$. We assume it has the form

$$r = R + \varepsilon\, S(R, \Theta, t) + O(\varepsilon^2) \quad ,$$
$$\nu = \Theta + \varepsilon\, T(R, \Theta, t) + O(\varepsilon^2) \quad , \tag{5}$$

and that the equations for R and Θ have the form

$$\dot{R} = \varepsilon\, F(R, \Theta, t) \quad , \quad \dot{\Theta} = \omega + \varepsilon\, G(R, \Theta, t). \tag{6}$$

We allow S and T to depend explicitly on the time t, because the equations of motion have explicit time dependence. Applying the transformation (5) to the original equations (2) and comparing the result with the assumed form (6) of the new equations, we find

$$LS = f(R, \Theta, t) - F(R, \Theta, t) \quad , \tag{7}$$

$$LT = g(R, \Theta, t) - G(R, \Theta, t) \quad , \tag{8}$$

where L is the directional derivative $L \equiv \frac{\partial}{\partial t} + \omega \frac{\partial}{\partial \Theta}$ along lines $\omega\Theta - t =$ constant of the t, Θ plane. We see that S and T will have secular terms proportional to t and Θ whenever there are non-zero components in the right hand sides of (7) and (8) that are constant along the lines $\omega\Theta - t =$ constant.

The suppression of such secular terms leads to natural choices for F and G. Consider the equation (7) for S. Inserting the explicit form of $f(R, \Theta, t)$ given by (3), it reads

$$LS = -\frac{R\omega'}{\omega} + \frac{r\omega'}{2\omega} \cos 2\Theta + \frac{a}{2\omega} \sin(t-\Theta) - \frac{a}{2\omega} \sin(t+\Theta) - F \quad . \tag{9}$$

We allow for the possibility of resonance, in which $\omega = 1$ for some range of time. During the time of resonance, L is the directional derivative along lines $\Theta - t = \text{constant}$. Hence, to avoid secular terms in S, we must choose F to suppress the terms $-\frac{R\omega'}{\omega}$ and $\frac{a}{2\omega}\sin(t-\Theta)$ from the right hand side of (9). That is,

$$F = -\frac{R\omega'}{\omega} + \frac{a}{2\omega}\sin(t-\Theta) \quad . \tag{10}$$

Similarly, suppression of secular terms in T leads to

$$G = -\frac{a}{2\omega R}\cos(t-\Theta) \quad . \tag{11}$$

With these choices of F and G, equations (7) and (8) can be integrated to find bounded values for S and T.

The equations for R and Θ are

$$\dot{R} = \varepsilon\{-\frac{R\omega'}{\omega} + \frac{a}{2\omega}\sin(t-\Theta)\} + O(\varepsilon^2) \quad , \tag{12}$$

$$\dot{\Theta} = \omega + \varepsilon\{-\frac{a}{2\omega R}\cos(t-\Theta)\} + O(\varepsilon^2) \quad . \tag{13}$$

If $a = 0$, (no forcing), then to leading order, (12) reads

$$\frac{\dot{R}}{R} = -\frac{\varepsilon\omega'}{2\omega} = -\frac{\dot{\omega}}{2\omega} \quad . \tag{14}$$

This equation integrates to

$$A \equiv R^2\,\omega = \text{constant} \quad . \tag{15}$$

The quantity A is the familiar adiabatic invariant. We introduce a change of variables $(R,\Theta) \to (A, \Psi \equiv \Theta - t)$ in equations (12) and (13). The equations for A and Ψ are

$$\dot{A} = \varepsilon a \omega^{-\frac{1}{2}} A^{\frac{1}{2}} \sin \Psi + O(\varepsilon^2) \quad , \tag{16}$$

$$\dot{\Psi} = \omega - 1 - \frac{\varepsilon a}{2} \omega^{-\frac{1}{2}} A^{-\frac{1}{2}} \cos \Psi + O(\varepsilon^2) \quad . \tag{17}$$

This system has explicit time dependence due to the presence of $\omega(\varepsilon t)$. Hence, a closed form solution is generally impossible. But an asymptotic solution can be constructed which is valid in near resonance conditions.

We take $\omega(\varepsilon t)$ to be a smooth function with $\omega(0) = 1$, $\omega'(0) = b$. Resonance occurs when t is near zero. (17) can be integrated to give

$$\Psi = \int_0^t \omega \, dt - t + O(\varepsilon t) = \frac{\varepsilon}{2} b \, t^2 + O(\varepsilon t + \varepsilon^2 t^3) \quad . \tag{18}$$

Let $t^* = \sqrt{\varepsilon} t$ be $O(1)$. Then

$$\Psi = \frac{b}{2} t^{*2} + O(\varepsilon^{\frac{1}{2}}) \quad . \tag{19}$$

Substituting this value of Ψ into (16) gives

$$A^{-\frac{1}{2}} \dot{A} = \varepsilon a \omega^{-\frac{1}{2}} (\sqrt{\varepsilon} \, t^*) \sin(\frac{b}{2} t^{*2}) + O(\varepsilon^{\frac{3}{2}}) =$$

$$\varepsilon a \sin(\frac{b}{2} t^{*2}) + O(\varepsilon^{\frac{3}{2}}) \quad . \tag{20}$$

Integration gives

$$A^{\frac{1}{2}} - A_0^{\frac{1}{2}} = \varepsilon a \int_0^t \sin(\frac{b}{2} t^{*2})dt + O(\varepsilon) =$$

$$\varepsilon^{\frac{1}{2}} a \int_0^{t^*} \sin(\frac{b}{2} \zeta^2)d\zeta + O(\varepsilon) \quad , \tag{21}$$

where A_0 is the value of A at $t = 0$. Since the total change of A is much less than unity, it is sufficient to approximate $A^{\frac{1}{2}} - A_0^{\frac{1}{2}}$ by $\frac{1}{2} A_0^{-\frac{1}{2}} \delta A$, where $\delta A \equiv A - A_0$. Hence,

$$\delta A = 2A_0^{\frac{1}{2}} \varepsilon^{\frac{1}{2}} a \int_0^{t^*} \sin(\frac{b}{2} t^{*2})dt^* + O(\varepsilon) \quad . \tag{22}$$

The total change in δA as t^* goes from $-\infty$ to $+\infty$ is

$$\left[\delta A\right]_{-\infty}^{+\infty} = 2A_0^{\frac{1}{2}} \varepsilon^{\frac{1}{2}} a \sqrt{\frac{\pi}{b}} \quad . \tag{23}$$

We see that the effect of the resonance is to alter the value of the adiabatic invariant by an amount $2A_0^{\frac{1}{2}} \varepsilon^{\frac{1}{2}} a \sqrt{\frac{\pi}{b}}$. This change occurs on a time scale $t = \frac{1}{\sqrt{\varepsilon}}$. Figure 3 shows a graph of δA vs. t^*.

CHAPTER 4

SLOWLY VARYING LIMIT CYCLES

1. Introduction

In many systems with limit cycles, the motion evolves to a stable periodic oscillation whose amplitude and frequency are fixed for all time. In this paper, we study the mechanism by which the motion of an autonomous system can approach a limit cycle on one time scale and then experience a further evolution away from this initial limit cycle on a longer time scale. The defining equations of the model are

$$\begin{aligned} \dot{r}_k &= \varepsilon\{A(r_1, r_2) + r_k \cos 2\nu_k\} \\ \dot{\nu}_k &= 1 + \varepsilon r_k \cos 2\nu_k \ , \ k = 1,2 \ , \end{aligned} \tag{1.1}$$

where $0 < \varepsilon << 1$ and the function $A(r_1, r_2)$ is assumed to be zero along some curve in the (r_1, r_2) plane. For a concrete example, we take

$$A(r_1, r_2) = - r_1 r_2\{(r_1 - 2)^2 + (r_2 - 2)^2 - 1\} \tag{1.2}$$

which is zero on the circle of radius 1 centered about $(r_1, r_2) = (2,2)$ and along the lines $r_1 = 0$ and $r_2 = 0$. We think of (1.1) as the polar form of a system that is originally given in rectangular variables. The rectangular variables (x_k, y_k) are related to the polar variables (r_k, ν_k) via

$$x_k = r_k \cos \nu_k, \; y_k = - r_k \sin \nu_k \; , \; k = 1,2 \quad . \tag{1.3}$$

Hence, r_k and ν_k represent the amplitudes and phases of oscillations in x_k and y_k. A limit cycle is achieved when the amplitudes r_1 and r_2 asymptote to constant values as $t \to \infty$.

In Section 2, we use the method of near identity transforms to derive equations for the long time evolution of the amplitudes r_1 and r_2, and in Section 3, we analyse these equations and compare the results with numerical calculations.

2. The Near Identity Transformation

We construct a near identity transformation $(r_k, \nu_k) \to (R_k, \Theta_k)$ so that the equations for the amplitudes R_1 and R_2 decouple from the phases Θ_1 and Θ_2. One can then study the two by two system of equations for R_1 and R_2 by phase plane methods. We assume that the transformation has the form

$$\begin{aligned} r_k &= R_k + \varepsilon \, S_k^1(R, \Theta) + \varepsilon^2 \, S_k^2(R, \Theta) + O(\varepsilon^3) \quad , \\ \nu_k &= \Theta_k + \varepsilon \, T_k^1(R, \Theta) + \varepsilon^2 \, T_k^2(R, \Theta) + O(\varepsilon^3) \quad , \end{aligned} \tag{2.1}$$

and that the equations in the new variables are

$$\begin{aligned} \dot{R}_k &= \varepsilon \, F_k^1(R, \Theta) + \varepsilon^2 \, F_k^2(R, \Theta) + O(\varepsilon^3) \quad , \\ \dot{\Theta}_k &= 1 + \varepsilon \, G_k^1(R, \Theta) + \varepsilon^2 \, G_k^2(R, \Theta) + O(\varepsilon^3) \; , \end{aligned} \tag{2.2}$$

Substituting (2.1) into the system (1.1) and comparing the result with (2.2), we find

$$LS_k^1 = A + R_k \cos 2\Theta_k - F_k^1 \quad , \tag{2.3}$$

$$LT_k^1 = R_k \cos 2\Theta_k - G_k^1 \quad , \tag{2.4}$$

$$LS_k^2 = \frac{\partial A}{\partial r_\ell} S_\ell^1 + \cos 2\Theta_k \, S_k^1 - 2R_k \sin 2\Theta_k \, T_k^1 - \frac{\partial S_k^1}{\partial R_\ell} F_\ell^1 - \frac{\partial S_k^1}{\partial \Theta_\ell} G_\ell^1 - F_k^2 \quad , \tag{2.5}$$

$$LT_k^2 = \cos 2\Theta_k \, S_k^1 - 2R_k \sin 2\Theta_k \, T_k^1 - \frac{\partial T_k^1}{\partial R_\ell} F_\ell^1 - \frac{\partial T_k^1}{\partial \Theta_\ell} G_\ell^1 - G_k^2 \quad , \tag{2.6}$$

where $L \equiv \frac{\partial}{\partial \Theta_1} + \frac{\partial}{\partial \Theta_2}$ is the directional derivative along the lines $\Theta_2 - \Theta_1 =$ constant of the (Θ_1, Θ_2) plane. In these equations, the function A and its derivatives are evaluated at $(r_1, r_2) = (R_1, R_2)$ and the index ℓ is summed over.

To suppress secular terms in S_k^1 and T_k^1, we balance F_k^1 and G_k^1 against terms in the right hand sides of (2.3) and (2.4) that are constant along the lines $\Theta_2 - \Theta_1 =$ constant. Hence, we choose

$$\begin{aligned} F_k^1(R_1, R_2) &= A(R_1, R_2) \quad , \\ G_k^1(R_1, R_2) &\equiv 0 \quad , \quad k = 1,2 \quad . \end{aligned} \tag{2.7}$$

With these choices of F_k^1 and G_k^1, (2.3) and (2.4) becomes

$$LS_k^1 = LT_k^1 = R_k \cos 2\Theta_k \ , \ k = 1,2 \ . \tag{2.8}$$

These equations have bounded solutions

$$S_k^1 = T_k^1 = \frac{R_k}{2} \sin 2\Theta_k \ , \ k = 1,2 \ . \tag{2.9}$$

Substituting the known values of F_k^1, G_k^1, S_k^1 and T_k^1 into (2.5) and (2.6), we find

$$LS_k^2 = \tfrac{1}{2}(R_\ell \frac{\partial A}{\partial r_\ell} - A) \sin 2\Theta_k + \frac{R_k}{4} \sin 4\Theta_k - \frac{R_k^2}{2}(1 - \cos 4\Theta_k) - F_k^2 \ , \tag{2.10}$$

$$LT_k^2 = -\frac{A}{2}(\sin 2\Theta_1 + \sin 2\Theta_2) + \frac{R_k}{4} \sin 4\Theta_k - \frac{R_k^2}{2}(1 - \cos 4\Theta_k) - G_k^2 \ . \tag{2.11}$$

Following the same procedure as before, we suppress secular terms in S_k^2 and T_k^2 by making the proper choices of F_k^2 and G_k^2. In the present case, it is sufficient to take

$$F_k^2 = G_k^2 = -\frac{R_k^2}{2} \ , \ k = 1,2 \ . \tag{2.12}$$

In $(\underset{\sim}{R}, \underset{\sim}{\Theta})$ variables, the equations of motion are

$$\begin{aligned} \dot{R}_1 &= \varepsilon\, A(R_1, R_2) - \varepsilon^2 \frac{R_1^2}{2} + O(\varepsilon^3) \\ \dot{R}_2 &= \varepsilon\, A(R_1, R_2) - \varepsilon^2 \frac{R_2^2}{2} + O(\varepsilon^3) \end{aligned} \tag{2.13}$$

and

$$\dot{\Theta}_k = 1 - \varepsilon^2 \frac{R_k^2}{2} + O(\varepsilon^3) \ , \ k = 1,2 \ . \tag{2.14}$$

Notice that the equations for the amplitudes R_1 and R_2 form a two by two system (2.13) decoupled from the phases Θ_1 and Θ_2. If we define the slow time $\tau = \varepsilon t$, then (2.13) can be written as

$$\begin{aligned} \frac{dR_1}{d\tau} &= A(R_1, R_2) - \varepsilon \frac{R_1^2}{2} + O(\varepsilon^2) \ , \\ \frac{dR_2}{d\tau} &= A(R_1, R_2) - \varepsilon \frac{R_2^2}{2} + O(\varepsilon^2) \ . \end{aligned} \tag{2.15}$$

3. The (R_1, R_2) Phase Plane

From (2.14), we see that the motion of the amplitudes R_1 and R_2 is described to $O(1)$ accuracy by the system

$$\frac{dR_1}{d\tau} = A(R_1, R_2) \ , \ \frac{dR_2}{d\tau} = A(R_1, R_2) \tag{3.1}$$

for slow time intervals of length $O(1)$ and by system

$$\begin{aligned} \frac{dR_1}{d\tau} &= A(R_1, R_2) - \varepsilon \frac{R_1^2}{2} \ , \\ \frac{dR_2}{d\tau} &= A(R_1, R_2) - \varepsilon \frac{R_2^2}{2} \ , \end{aligned} \tag{3.2}$$

for slow time intervals of length $O(\frac{1}{\varepsilon})$. Figure 4.1 shows the phase portrait of (3.1). The trajectories all have slope + 1. Inside the circle $(R_1 - 2)^2 + (R_2 - 2)^2 = 1$, $A(R_1, R_2) = - R_1 R_2\{(R_1 - 2)^2 + (R_2 - 2)^2 - 1\} > 0$, so R_1 and R_2 increase at the same rate. Outside the circle, $A < 0$, so R_1 and R_2 decrease at the same rate. The circle itself is a locus of singular points. The solid semicircle C_+ represents the stable singular points and the broken semicircle C_- represents the unstable singular points. The shaded region S shows the trajectories that converge to the stable singular points.

Figure 4.2 shows the phase portrait of (3.2). The $O(\varepsilon)$ terms which are present in (3.2) but not in (3.1) introduce an essential change. The system (3.2) has only 3 singular points. These are located at $(R_1, R_2) = (0, 0)$, (R_L, R_L) and (R_U, R_U), where R_L and R_U are the two positive roots of $A(R, R) - \varepsilon \frac{R^2}{2} = 0$. Since $A(R, R) = 0$ has roots $0, 2 - \frac{1}{\sqrt{2}}$ and $2 + \frac{1}{\sqrt{2}}$, we have $R_L = 2 - \frac{1}{\sqrt{2}} + O(\varepsilon)$ and $R_U = 2 + \frac{1}{\sqrt{2}} + O(\varepsilon)$. The singular point (R_U, R_U) is a stable node. All trajectories enter the node with slope - 1, except one, which enters with slope unity. The singular point (R_L, R_L) is a saddle. The two outgoing solutions depart from the saddle point with slope 1, and the two ingoing solutions enter with slope - 1. The shaded region $\bar{S}$ shows the trajectories that converge to the stable node.

Let us consider the motion along a typical trajectory in $\bar{S}$. Initially, $A(R_1, R_2)$ is $O(1)$ and the motion is described to $O(1)$ accuracy by (3.1). The phase point travels toward the semicircle C_+ along a trajectory with slope nearly unity. This phase of the journey occurs on a slow time scale $\tau = O(1)$. When the phase point is within

distance $O(\varepsilon)$ of C_+, the whole right hand side of (3.2) is $O(\varepsilon)$. The phase point drifts to the stable node on a slow time scale $O(\frac{1}{\varepsilon})$.

We now consider the implications of these results regarding the oscillations in the original variables x_k, y_k, $k = 1,2$. Once the R_k are known, we find the amplitudes r_k of the oscillations in x_k and y_k via $r_k = R_k(\varepsilon t) + O(\varepsilon)$. Hence, we see that the oscillations in x_k, y_k, $k = 1,2$ appear to approach limit cycles in time $t = O(\frac{1}{\varepsilon})$, yet experience a further evolution away from their initial limit cycles in time $t = O(\frac{1}{\varepsilon^2})$.

We compare the results of the theory with a numerical simulation. Figure 4.3 shows the trajectory of the amplitudes r_1 and r_2 obtained from a numerical solution of (1.1) with $\varepsilon = .05$. The initial conditions are $r_1 = 4$, $r_2 = 2.5$, $v_1 = v_2 = 0$. The segment AB represents the initial formation of the limit cycles and the segment BC represents the slow drift away from the initial limit cycles. The elapsed times for these motions are 8.2 and 380, in good agreement with $\frac{1}{\varepsilon} = 20$ and $\frac{1}{\varepsilon^2} = 400$, which are the natural time scales determined from the theory.

Part II

NONLINEAR CHEMICAL OSCILLATIONS IN DISCRETE AND CONTINUOUS SYSTEMS

CHAPTER 5

CHEMICAL WAVES

1. Introduction

We study the propagation of chemical waves through a continuous diffusive medium. These arise naturally and as models for biochemical processes. Motivated by specific experimental results of M. Marek and E. Svobodova [3], we initiate our study with the investigation of a reaction diffusion process governed by the equations

$$\begin{aligned} \frac{\partial x}{\partial t} &= F(x, y) + \varepsilon \frac{\partial^2 x}{\partial s^2} \quad , \\ \frac{\partial y}{\partial t} &= G(x, y) + \varepsilon \frac{\partial^2 y}{\partial s^2} \quad , \end{aligned} \tag{1.1}$$

where $0 < \varepsilon << 1$.

When $\varepsilon = 0$, oscillations at any spatial position s are governed by

$$\begin{aligned} \overset{o}{x} &= F(x, y) \\ \overset{o}{y} &= G(x, y) \quad . \end{aligned} \tag{1.2}$$

We assume that as $t \to \infty$, all solutions of (1.2) tend to a stable, T periodic limit cycle given by

$$x = X(t) \ , \ y = Y(t) \quad . \tag{1.3}$$

Our major result is that to leading order in ε the system (1.1) possesses

a periodic wave solution given by

$$x = X(t + \Psi(s, \tau)) \ , \ y = Y(t + \Psi(s, \tau)) \ , \tag{1.4}$$

where $\tau = \varepsilon t$ and the phase $\Psi(s, \tau)$ evolves according to the nonlinear equation

$$\frac{\partial \Psi}{\partial \tau} = \frac{\partial^2 \Psi}{\partial s^2} - \frac{\kappa}{2} \left(\frac{\partial \Psi}{\partial s}\right)^2 \ . \tag{1.5}$$

Hence, the gradient of the phase $v \equiv \frac{\partial \Psi}{\partial s}$ obeys Burger's equation [4]

$$\frac{\partial v}{\partial t} + \kappa v \frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial s^2} \ . \tag{1.6}$$

These results are derived in Section 3. Prior to the derivation we shall need specific preliminary results which are implied by the assumption that (1.2) possesses a stable, T periodic limit cycle. These are derived in Section 2.

Our results have many implications regarding the propagation of chemical waves in a diffusive medium. These are discussed in Section 4. One of the specific tasks is to account for the experimental observations of Marek and Svobodova [3] on the Belusov-Zhabotinskii reaction.

2. The New Variables

At any given position s, we expect that the $O(\varepsilon)$ diffusion terms in (1.1) will cause the orbit of $(x(s, t)), y(s, t))$ to suffer $O(\varepsilon)$ displacements from the trajectory of the limit cycle given in (1.2).

The consideration suggests a convenient change of variable $(x, y) \to (A, \Theta)$ given by

$$\begin{aligned} x &= X(\Theta) + \varepsilon A Y'(\Theta) \quad , \\ y &= Y(\Theta) - \varepsilon A X'(\Theta) \quad . \end{aligned} \tag{2.1}$$

Here, Θ parametrizes points on the limit cycle and εA measures perpendicular displacements from the limit cycle. Figure 5.1 provides a geometric visualization of this transformation.

Applying the transformation $(x, y) \to (A, \Theta)$ to the full reaction diffusion system (1.1), we find

$$\begin{aligned} \frac{\partial A}{\partial t} &= \varphi(\Theta)A + Q(\Theta)\left(\frac{\partial \Theta}{\partial s}\right)^2 + \varepsilon U + O(\varepsilon^2) \quad , \\ \frac{\partial \Theta}{\partial t} &= 1 + \varepsilon\{\gamma(\Theta)A + P(\Theta)\left(\frac{\partial \Theta}{\partial s}\right)^2 + \frac{\partial^2 \Theta}{\partial s^2}\} + O(\varepsilon^2) \quad . \end{aligned} \tag{2.2}$$

Here, φ, γ, Q, P are functions of Θ determined from $X(\Theta)$ and $Y(\Theta)$, and U is a function of A, Θ and their s derivatives. The specific functional forms of these quantities is not crucial for the analysis. It is sufficient to note that they are all T periodic in Θ and that

$$\int_0^T \varphi(\zeta)d\zeta < 0 \quad , \tag{2.3}$$

which derives from the stability of the limit cycle (1.3).

To derive (2.3), we consider space independent solutions of (2.2), with $\frac{\partial \Theta}{\partial s}$, $\frac{\partial A}{\partial s}$ equal to zero. They satisfy

$$\frac{dA}{dt} = \varphi(\Theta)A + O(\varepsilon) \quad ,$$
$$\frac{d\Theta}{dt} = 1 + O(\varepsilon) \quad . \tag{2.4}$$

From (2.4), we deduce

$$\frac{dA}{dt} = \varphi(t)A + O(\varepsilon) \tag{2.5}$$

for time intervals with length $O(1)$. Integration of (2.5) gives

$$\frac{A(t+T)}{A(t)} = (1 + O(\varepsilon))e^{\int_0^T \varphi(\zeta)d\zeta} \tag{2.6}$$

Here, we used the periodicity of φ to change $\int_t^{t+T} \varphi(\zeta)d\zeta$ into $\int_0^T \varphi(\zeta)d\zeta$. In (A, Θ) coordinates, the limit cycle is given by $A \equiv 0$, $\Theta = t + \Psi$. Stability of the limit cycle means that all solutions of (2.4) have $A(t) \to 0$ as $t \to \infty$. From (2.6), we see that this requirement forces the condition

$$\int_0^T \varphi(\zeta)d\zeta < 0 \quad .$$

3. The Two Timing Procedure

We show that to leading order, the asymptotic solution of the system (2.2) has

$$\Theta \sim t + \Psi(s, \tau) \quad , \tag{3.1}$$

where τ is the slow time εt and the phase $\Psi(s, \tau)$ evolves according to

$$\frac{\partial \Psi}{\partial \tau} = \frac{\partial^2 \Psi}{\partial s^2} - \frac{\kappa}{2} \left(\frac{\partial \Psi}{\partial s}\right)^2 \quad . \tag{3.2}$$

Given Ψ, we find the asymptotic solutions for the concentrations x and y via the transformation (2.1):

$$\begin{aligned} x &= X(\Theta) + \varepsilon A Y'(\Theta) = A(t + \Psi) + O(\varepsilon) \quad , \\ y &= Y(\Theta) - \varepsilon A X'(\Theta) = Y(t + \Psi) + O(\varepsilon) \quad . \end{aligned} \tag{3.3}$$

We seek an asymptotic solution of (2.2) in the form

$$A \sim A^0 + \varepsilon A^1 \quad , \quad \Theta \sim \Theta^0 + \varepsilon \Theta^1 \quad , \tag{3.4}$$

where the terms in the expansion depend on t, s and the slow time $\tau = \varepsilon t$. Substituting (3.4) into (2.2), we obtain the hierarchy

$O(1)$

$$\frac{\partial A^0}{\partial t} - \varphi(\Theta^0) A^0 = Q(\Theta^0) \left(\frac{\partial \Theta^0}{\partial s}\right)^2 \quad , \tag{3.5a}$$

$$\frac{\partial \Theta^0}{\partial t} = 1 \quad , \tag{3.5b}$$

$O(\varepsilon)$

$$\frac{\partial A^1}{\partial t} - \varphi(\Theta^0)A^1 = \{\varphi'(\Theta^0)A^0 + Q'(\Theta^0)(\frac{\partial \Theta^0}{\partial s})^2\}\Theta' + 2Q(\Theta^0)\frac{\partial \Theta^0}{\partial s}\frac{\partial \Theta^1}{\partial s} + U \qquad (3.5c)$$

$$\frac{\partial \Theta^1}{\partial t} = \gamma(\Theta^0)A^0 + P(\Theta^0)(\frac{\partial \Theta^0}{\partial s})^2 + \frac{\partial^2 \Theta^0}{\partial s^2} - \frac{\partial \Theta^0}{\partial \tau} \quad . \qquad (3.5d)$$

From (3.5b), we find

$$\Theta^0 = t + \Psi(s, \tau) \quad . \qquad (3.6)$$

Substituting this value of Θ^0 into (3.5a), we find

$$\frac{\partial A^0}{\partial t} - \varphi(t + \Psi)A^0 = Q(t + \Psi)(\frac{\partial \Psi}{\partial s})^2 \quad . \qquad (3.7)$$

To solve (3.7), we consider the equation

$$\frac{dx}{d\zeta} - \varphi(\zeta)x = Q(\zeta) \quad . \qquad (3.8)$$

This is a linear ODE with T periodic coefficients and T periodic forcing. The homogeneous solution

$$h = h_0 e^{V(\zeta)} \ , \ V(\zeta) \equiv \int_0^\zeta \varphi(\zeta)d\zeta \qquad (3.9)$$

is a decaying transient because of the condition $\int_0^T \varphi(\zeta)d\zeta < 0$, which derived from the stability of the limit cycle. Under these conditions, (3.8) has a unique periodic solution $\rho(\zeta)$ [5]. In terms of this $\rho(\zeta)$, the general solution of (3.7) is

$$A^0 = h_0(\tau)e^{V(t)} + \left(\frac{\partial\Psi}{\partial s}\right)^2 \rho(t + \Psi)$$
$$= h_0(\tau)e^{V(t)} + \left(\frac{\partial\Psi}{\partial s}\right)^2 \rho(\Theta^0) \quad . \tag{3.10}$$

Substituting this result for A^0 into (3.5d) gives

$$\frac{\partial\Theta^1}{\partial t} = \gamma(\Theta^0)h_0(\tau)e^{V(t)} + \{\gamma(\Theta^0)\rho(\Theta^0) + P(\Theta^0)\}\left(\frac{\partial\Psi}{\partial s}\right)^2 + \frac{\partial^2\Psi}{\partial s^2} - \frac{\partial\Psi}{\partial s} \quad . \tag{3.11}$$

This function $f(\Theta^0) \equiv \gamma(\Theta^0)\rho(\Theta^0) + P(\Theta^0)$ is T periodic, hence, we can write it in the form

$$f(\Theta^0) = -\frac{\kappa}{2} + \omega(\Theta^0) \quad , \tag{3.12}$$

where $\kappa = -\frac{2}{T}\int_0^T f(\zeta)d\zeta$ and $\omega(\Theta^0)$ is T periodic with zero mean value. Hence (3.11) integrates to

$$\Theta^1 = \{\frac{\partial^2\Psi}{\partial s^2} - \frac{\partial\Psi}{\partial\tau} - \frac{\kappa}{2}\left(\frac{\partial\Psi}{\partial s}\right)^2\}t + h_0(\tau)\int^t \gamma(\Theta^0)e^{V(t)}dt + \left(\frac{\partial\Psi}{\partial s}\right)^2\int^t \omega(\Theta^0)dt. \tag{3.13}$$

The second term is bounded because $\gamma(\Theta^0)e^{V(t)}$ decays exponentially as $t \to \infty$. The third term is bounded because $\omega(\Theta^0)$ is periodic with zero mean value. Hence, we write

$$\Theta^1 = \mu(\Psi)t + B(t, \tau) \quad , \tag{3.14}$$

where

$$\mu(\Psi) \equiv \frac{\partial^2\Psi}{\partial s^2} - \frac{\partial\Psi}{\partial\tau} - \frac{\kappa}{2}\left(\frac{\partial\Psi}{\partial s}\right)^2 \tag{3.15}$$

and $B(t, \tau)$ is a bounded function composed of periodic and exponentially decaying terms. The equation for A^1 is obtained by substituting the result (3.14) for Θ^1 into (3.5c). The result can be expressed as

$$\frac{\partial A^1}{\partial t} - \varphi(\Theta^0)A^1 + B(t, \tau) = \{\mu(\Psi)W(\Theta^0) \frac{\partial \Psi}{\partial s} + 2Q(\Theta^0) \frac{\partial}{\partial s} \mu(\Psi)\}\frac{\partial \Psi}{\partial s} t \quad (3.16)$$

where $B(t, \tau)$ is another bounded function composed of periodic and exponentially decaying terms and

$$W(\Theta^0) \equiv \varphi'(\Theta^0) \rho(\Theta^0) + Q'(\Theta^0) \quad . \quad (3.17)$$

For a physically meaningful solution, the amplitude correction A^1 and its time derivative $\frac{\partial A^1}{\partial t}$ must remain bounded for all time. If this is the case, then (3.16) forces us to conclude that

$$\{\mu(\Psi)\ W(\Theta^0) \frac{\partial \Psi}{\partial s} + 2Q(\Theta^0) \frac{\partial}{\partial s} \mu(\Psi)\} \frac{\partial \Psi}{\partial s} t \quad (3.18)$$

is bounded. In general, $W(\Theta^0)$ and $Q(\Theta^0)$ are two different periodic functions of t. Hence, the boundedness of (3.18) implies $\frac{\partial \Psi}{\partial s} \equiv 0$ or $\mu(\Psi) \equiv 0$. The first alternative, $\frac{\partial \Psi}{\partial s} \equiv 0$, corresponds to solutions that are space independent to leading order. For spatially dependent solutions, we must have

$$\mu(\Psi) \equiv \frac{\partial^2 \Psi}{\partial s^2} - \frac{\partial \Psi}{\partial \tau} - \frac{\kappa}{2} (\frac{\partial \Psi}{\partial s})^2 = 0 \quad , \quad (3.20)$$

this is the main result.

Differentiating (3.20) with respect to s and setting $v = \frac{\partial \Psi}{\partial s}$ gives

$$\frac{\partial v}{\partial \tau} + \kappa v \frac{\partial v}{\partial s} = \frac{\partial^2 v}{\partial s^2} \quad , \tag{3.21}$$

which is the well known Burger's equation. Like Burger's equation, (3.20) admits an exact linearization. Under the transformation

$$\Psi = - \frac{2}{\kappa} \log \varphi \quad , \tag{3.22}$$

(3.23) becomes the ordinary heat equation

$$\frac{\partial \varphi}{\partial \tau} \quad \frac{\partial^2 \varphi}{\partial s^2} \quad . \tag{3.23}$$

4. Propagation of Chemical Waves

Given a solution $\Psi(s, \tau)$ of (3.20), we determine asymptotic solutions for x and y via

$$x \sim X(t + \Psi(s, \tau)) \quad , \quad y \sim Y(t + \Psi(s, \tau)) \quad . \tag{4.1}$$

Near any given point s, the solution looks like a travelling wave with frequency $\simeq \frac{2\pi}{T}$ and wave number $\frac{2\pi}{T} \frac{\partial \Psi}{\partial s}$. Hence, (3.21) tells us that the wave number evolves slowly in time according to Burger's equation. A well known solution of Burger's equation (3.21) is the single shock

$$v = v_1 + \frac{v_2 - v_1}{1 + \exp\{\frac{\kappa(v_2 - v_1)}{2} (s - U\tau)\}} \tag{4.2}$$

where $U = \frac{1}{2}(v_1 + v_2)$. This solution has

$$v \sim \begin{cases} v_1 & \text{as} \quad s - U\tau \to +\infty \\ v_2 & \text{as} \quad s - U\tau \to -\infty \end{cases} . \tag{4.3}$$

The corresponding wave train of chemical concentrations has wave number $\frac{2\pi}{T} v_1$ as $s - U\tau \to +\infty$ and wave number $\frac{2\pi}{T} v_2$ as $s - U\tau \to -\infty$. The shock, or transition between these two values of wave number occurs at $s - U\tau = s - \varepsilon Ut = 0$. Hence, the shock moves with speed εU. Figure 5.2 provides a visualization of the solution for x at a fixed instant of time.

We now turn to the experiment of Marek and Svobodova. Their apparatus consists of a tubular reactor which has one end attached to a continuous stirred tank reactor. Figure 5.3 shows the experimental set up. In each reactor, Belusov-Zhabotinskii reactions with slightly different parameters are taking place. Initially, the concentrations in the tubular reactor are spatially uniform. The continuous stirred tank reactor acts as a forcing at one end of the tubular reactor. When the forcing is turned on, chemical concentration waves propagate into the tubular reactor, until finally, there are waves traversing its whole length.

We model the oscillations in the tubular reactor by the reaction diffusion system

$$\begin{aligned} \frac{\partial x}{\partial t} &= F(x, y) + \varepsilon \frac{\partial^2 x}{\partial s^2} , \\ \frac{\partial y}{\partial t} &= G(x, y) + \varepsilon \frac{\partial^2 y}{\partial s^2} . \end{aligned} \tag{4.4}$$

x and y are initially uniform in space, undergoing oscillations only in time. Let us take $x(s, 0) = X(0)$, $y(s, 0) = Y(0)$ for initial conditions in $s > 0$. We model the effect of the CSTR's forcing at the end $s = 0$ by the boundary conditions $x(0, t) = X(\{1 + \varepsilon\omega\}t)$, $y(0, t) = Y(\{1 + \varepsilon\omega\}t)$. In words, at the end $s = 0$, one sees limit cycle oscillations with a period slightly different from T. This is due to choice. The parameters of the CSTR and the tube reactor are slightly different.

The boundary value, initial value problem for the phase $\Psi(s, \tau)$ in the asymptotic solution (4.1) is

$$\frac{\partial \Psi}{\partial \tau} = \frac{\partial^2 \Psi}{\partial s^2} - \frac{\kappa}{2}\left(\frac{\partial \Psi}{\partial s}\right)^2 \quad \text{in} \quad s > 0$$

$$\Psi(s, 0) = 0 \ , \ \Psi(0, \tau) = \omega\tau \quad . \tag{4.5}$$

The corresponding problem for $\varphi = e^{-\frac{1}{2}\kappa\Psi}$ is

$$\frac{\partial \varphi}{\partial \tau} = \frac{\partial^2 \varphi}{\partial s^2} \quad \text{in} \quad s > 0$$

$$\varphi(s, 0) = 1 \ , \ \varphi(0, \tau) = e^{-\frac{1}{2}\kappa\omega\tau} \quad . \tag{4.6}$$

This standard problem is easily solved. We omit the details and present the results. A solution that corresponds to a propagating wave occurs when $W \equiv -\kappa\omega > 0$. For $W\tau >> \sqrt{W}s$, the solution approaches the elementary separation of variables solution

$$e^{\frac{1}{2}(W\tau - \sqrt{W}s)} \quad . \tag{4.7}$$

For $W\tau << \sqrt{W}s$, the solution approaches unity, the value given at $\tau = 0$. Hence, the phase Ψ is given by

$$\Psi \sim \begin{cases} \frac{1}{\kappa} (\sqrt{W}s - W\tau) , & W\tau >> \sqrt{W}s , \\ 0 , & W\tau << \sqrt{W}s , \end{cases} \tag{4.8}$$

and the wave number is proportional to

$$v = \frac{\partial \Psi}{\partial s} \sim \begin{cases} \frac{1}{\kappa} \sqrt{W} , & W\tau >> \sqrt{W}s , \\ 0 , & W\tau << \sqrt{W}s . \end{cases} \tag{4.9}$$

The corresponding solution for the chemical concentration $x(s, t)$ looks like a wave train with wave number $\frac{2\pi}{T} \cdot v = \frac{2\pi}{\kappa T} \sqrt{W}$ for $W\tau >> \sqrt{W}s$, and like a spatially independent oscillation in time for $W\tau << \sqrt{W}s$. Figure 5.4 summarizes these results.

CHAPTER 6

COUPLED CHEMICAL OSCILLATORS

1. Introduction

We study the time evolution of two coupled chemical oscillators. Systems of coupled chemical oscillators arise naturally and as models of time periodic processes in living organisms. Motivated by observations of Marek and Stuchl [6] on the Belusov-Zhabotinskii reaction, we study the system

$$\begin{aligned}
\dot{x}_1 &= F(x_1, y_1) + \varepsilon\{k(x_2 - x_1) + \lambda\, f(x_1, y_1)\} \\
\dot{y}_1 &= G(x_1, y_1) + \varepsilon\{k(y_2 - y_1) + \lambda\, g(x_1, y_1)\} \\
\dot{x}_2 &= F(x_2, y_2) + \varepsilon\, k(x_1 - x_2) \\
\dot{y}_2 &= G(x_2, y_2) + \varepsilon\, k(y_1 - y_2) \quad ,
\end{aligned} \tag{1.1}$$

where $0 < \varepsilon << 1$. The parameter k is a positive coupling constant. When $\varepsilon = 0$, we have two identical uncoupled oscillators described by

$$\begin{aligned}
\dot{x}_i &= F(x_i, y_i) \\
\dot{y}_i &= G(x_i, y_i) \quad , \; i = 1,2 \quad .
\end{aligned} \tag{1.2}$$

We assume that (1.2) has a stable, T-periodic limit cycle given by

$$x_i = X(t + \Psi_i) \quad , \quad y_i = Y(t + \Psi_i) \quad , \; i = 1,2 \quad , \tag{1.3}$$

where the Ψ_i are arbitrary constants. When $\lambda = 0$, $\varepsilon \neq 0$, two

identical oscillators are coupled. When $\lambda \neq 0$, $\varepsilon \neq 0$, two different oscillators are coupled. Notice that the forcing of the oscillators upon each other is proportional to the differences $x_2 - x_1$ and $y_2 - y_1$. This derives from the physical assumption that the coupling is due to mass transfer.

Using multiscale asymptotics, we show that to lowest order in ε, the solution of (1.1) is

$$x_i = X(t + \Psi_i(\tau)) \ , \ y_i = Y(t + \Psi_i(\tau)) \ , \ i = 1,2 \ , \tag{1.4}$$

where $\tau = \varepsilon t$ and the phase shift $\bar{\Psi}(\tau) \equiv \Psi_2(\tau) - \Psi_1(\tau)$ satisfies

$$\frac{d\bar{\Psi}}{d\tau} = k \, P(\bar{\Psi}) + \lambda\beta \ . \tag{1.5}$$

Here, β is a constant determined from certain integrals involving the functions X, Y, f and g, and $P(\bar{\Psi})$ is a T-periodic function determined from X and Y which has value 0 and slope -2 when $\bar{\Psi}$ is an integer multiple of T.

The theory has significant implications regarding coupled chemical oscillators. The observed coupling phenomena and their bifurcations can be explained by the evolution of the phase shift $\bar{\Psi}(\tau)$. These topics are pursued in Section 3. In particular, we account for experimental observations by M. Marek and I. Stuchl [6] on coupled Belusov-Zhabotinskii reactions; in particular, we account for synchronization and its bifurcation into rhythm-splitting.

2. The Perturbation Theory

It is convenient to change from the variables x_i, $y_i (i = 1,2)$ to the variables A_i, $\Theta_i (i = 1,2)$ by means of the transformation

$$\begin{aligned} x_i &= X(\Theta_i) + \varepsilon A_i Y'(\Theta_i) \quad , \\ y_i &= Y(\Theta_i) - \varepsilon A_i X'(\Theta_i) \quad , \quad i = 1,2 \ . \end{aligned} \tag{2.1}$$

Here, Θ_i parametrizes points on the limit cycle and A_i measures displacements perpendicular to the limit cycle. A more complete discussion of this transformation is given in Chapter 5. In A_i, Θ_i coordinates, the system (1.1) becomes

$$\begin{aligned} \dot{A}_1 &= \Phi(\Theta_1)A_1 + kU(\Theta_1, \Theta_2) + \lambda\varphi(\Theta_1) + \varepsilon u_1(\underset{\sim}{A}, \underset{\sim}{\Theta}) + O(\varepsilon^2) \quad , \\ \dot{\Theta}_1 &= 1 + \varepsilon\{\Gamma(\Theta_1)A_1 + \lambda\gamma(\Theta_1) + kr(\Theta_1) + kV(\Theta_1, \Theta_2)\} + O(\varepsilon^2) \quad , \\ \dot{A}_2 &= \Phi(\Theta_2)A_2 + kU(\Theta_2, \Theta_1) + \varepsilon u_2(\underset{\sim}{A}, \underset{\sim}{\Theta}) + O(\varepsilon_2) \quad , \\ \dot{\Theta}_2 &= 1 + \varepsilon\{\Gamma(\Theta_2)A_2 + kr(\Theta_2) + kV(\Theta_2, \Theta_1)\} + O(\varepsilon^2) \quad . \end{aligned} \tag{2.2}$$

In these, $U(\Theta_1, \Theta_2)$ and $V(\Theta_1, \Theta_2)$ are related to X and Y via

$$U(\Theta_1, \Theta_2) = \{X(\Theta_2) Y'(\Theta_1) - Y(\Theta_2) X'(\Theta_1)\}/R^2(\Theta_1) \tag{2.3a}$$

$$V(\Theta_1, \Theta_2) = \{X(\Theta_2) X'(\Theta_1) + Y(\Theta_2) Y'(\Theta_1)\}/R^2(\Theta_1) \quad , \tag{2.3b}$$

where $R^2(\Theta) = X'^2(\Theta) + Y'^2(\Theta)$. The exact forms of the remaining functions Φ, φ, P, γ, r, u_1 and u_2 are not crucial for this analysis. It is sufficient to note that they are all T-periodic in Θ_1 and Θ_2 and that

$$\int_0^T \Phi(\zeta)d\zeta < 0 \quad , \tag{2.4}$$

which derives from the stability of the limit cycle. The details of the argument leading to (2.4) are given in Chapter 5.

We show that to leading order in ε, the asymptotic solution of the system (2.2) has

$$\Theta_i = t + \Psi_i(\tau) \quad , \tag{2.5}$$

where the phases $\Psi_i(\tau)$ satisfy

$$\frac{d\Psi_1}{d\tau} = H(\Psi_2 - \Psi_1) + \lambda\beta \quad , \tag{2.6a}$$

$$\frac{d\Psi_2}{d\tau} = H(\Psi_1 - \Psi_2) \quad . \tag{2.6b}$$

Here, H is a T-periodic function with slope one at $\bar{\Psi} = 0$. Subtracting (2.6b) from (2.6a) gives the equation for the phase shift $\bar{\Psi} = \Psi_2 - \Psi_1$,

$$\frac{d\bar{\Psi}}{d\tau} = kP(\bar{\Psi}) - \lambda\beta \quad , \tag{2.7}$$

where $P(\bar{\Psi}) \equiv H(-\bar{\Psi}) - H(\bar{\Psi})$. Once the $\Psi_i(\tau)$ are determined, we find the solution for x_i and y_i from the transformation (2.1):

$$\begin{aligned} x_i(t) &= X(\Theta_i) + \varepsilon A_i Y'(\Theta_i) = X(t + \Psi_i(\tau)) + O(\varepsilon) \quad , \\ y_i(t) &= Y(\Theta_i) - \varepsilon A_i X'(\Theta_i) = Y(t + \Psi_i(\tau)) + O(\varepsilon) \quad . \end{aligned} \tag{2.8}$$

We seek an asymptotic solution of (2.2) in the form

$$A_i \sim A_i^0 + \varepsilon A_i^1 \ , \ \Theta_i = \Theta_i^0 + \varepsilon \Theta_i^1 \ , \tag{2.9}$$

where the terms in the expansion depend on t and $\tau = \varepsilon t$. Substituting (2.9) into (2.2), we obtain a hierarchy

$O(1)$

$$\frac{\partial A_1^0}{\partial t} - \Phi(\Theta_1^0)A_1^0 = kU(\Theta_1^0, \Theta_2^0) + \lambda\Psi(\Theta_1^0) \tag{2.10a}$$

$$\frac{\partial \Theta_1^0}{\partial t} = 1 \ , \tag{2.10b}$$

$$\frac{\partial A_2^0}{\partial t} - \Phi(\Theta_2^0)A_2^0 = kU(\Theta_2^0, \Theta_1^0) \ , \tag{2.10c}$$

$$\frac{\partial \Theta_2^0}{\partial t} = 1 \ . \tag{2.10d}$$

$O(\varepsilon)$

$$\frac{\partial A_1^1}{\partial t} - \Phi(\Theta_1^0)A_1^1 = \{\Phi'(\Theta_1^0)A_1^0 + k\frac{\partial U}{\partial \Theta_1}(\Theta_1^0, \Theta_2^0) + \lambda\Psi'(\Theta_1^0)\}\Theta_1^1 \tag{2.11a}$$

$$+ k\frac{\partial U}{\partial \Theta_2}(\Theta_1^0, \Theta_2^0)\Theta_2^1 + u_1(\underset{\sim}{A}^0, \underset{\sim}{\Theta}^0) - \frac{\partial A_1^0}{\partial \tau}$$

$$\frac{\partial \Theta_1^1}{\partial t} = \Gamma(\Theta_1^0)A_1^0 + \lambda\gamma(\Theta_1^0) + kr(\Theta_1^0) + kV(\Theta_1^0, \Theta_2^0) - \frac{\partial \Theta_1^0}{\partial \tau} \tag{2.11b}$$

$$\frac{\partial A_2^1}{\partial t} - \Phi(\Theta_2^0)A_2^1 = \{\Phi'(\Theta_2^0)A_2^0 + k\frac{\partial U}{\partial \Theta_1}(\Theta_2^0, \Theta_1^0)\}\Theta_2^1 \tag{2.11c}$$

$$+ k\frac{\partial U}{\partial \Theta_2}(\Theta_2^0, \Theta_1^0)\Theta_1^1 + u_2(\underset{\sim}{A}^0, \underset{\sim}{\Theta}^0) - \frac{\partial A_2^0}{\partial \tau} \ .$$

$$\frac{\partial \Theta_2^1}{\partial t} = \Gamma(\Theta_2^0)A_2^0 + kV(\Theta_2^0, \Theta_1^0) - \frac{\partial \Theta_2^0}{\partial \tau} \ . \tag{2.11d}$$

From (2.10b,d), we find

$$\Theta_i^0 = t + \Psi_i(\tau) \ , \ i = 1,2 \ . \tag{2.12}$$

Substituting these values of Θ_i^0 into (2.10a,c) gives

$$\frac{\partial A_1^0}{\partial t} - \Phi(t + \Psi_1)A_1^0 = kU(t + \Psi_1, \ t + \Psi_2) + \lambda\varphi(t + \Psi_1) \tag{2.13a}$$

$$\frac{\partial A_2^0}{\partial t} - \Phi(t + \Psi_2)A_2^0 = kU(t + \Psi_2, \ t + \Psi_1) \ . \tag{2.13b}$$

To solve (2.13a,b), we consider the equations

$$\frac{dx}{d\zeta} - \Phi(\zeta)x = \varphi(\zeta) \tag{2.14a}$$

$$\frac{dy}{d\zeta} - \Phi(\zeta)y = U(\zeta, \ \zeta + \bar{\Psi}) \ , \tag{2.14b}$$

where $\bar{\Psi} \equiv \Psi_2 - \Psi_1$. These are first order, linear ODE's with periodic coefficients and forcing. In each case, the homogeneous solution

$$e^{v(\zeta)} \ , \ v(\zeta) \equiv \int_0^\zeta \Phi(\zeta)d\zeta$$

is a decaying transient because of the condition $\int_0^T \phi(\zeta)d\zeta < 0$, which derives from the stability of the limit cycles. Under these conditions, (2.14a,b) have unique T-periodic solutions

$$x = p(\zeta) \ , \ y = \rho(\zeta, \bar{\Psi}) \ . \tag{2.15}$$

In terms of $\rho(\zeta)$ and $\rho(\zeta, \underline{\bar{\Psi}})$, the general solutions of (2.13a,b) are

$$A_1^0 = k\rho(t + \Psi_1, \underline{\bar{\Psi}}) + \lambda p(t + \Psi_1) + h_1(\tau)e^{v(t + \Psi_1)} \tag{2.16a}$$

$$A_2^0 = k\rho(t + \Psi_2, -\underline{\bar{\Psi}}) + h_2(\tau)e^{v(t + \Psi_2)} \quad . \tag{2.16b}$$

Substituting these into (2.11b,d), we find

$$\frac{\partial \Theta_1^1}{\partial t} = \{k\rho(t + \Psi_1, \underline{\bar{\Psi}}) + \lambda p(t + \Psi_1)\}\, \Gamma(t + \Psi_1) + \lambda\gamma(t + \Psi_1) + \tag{2.17a}$$

$$kr(t + \Psi_1) + kV(t + \Psi_1,\ t + \Psi_2) - \frac{d\Psi_1}{d\tau} + h_1(\tau)e^{v(t + \Psi_1)}\, \Gamma(t + \Psi_1) \quad ,$$

$$\frac{\partial \Theta_2^1}{\partial t} = k\rho(t + \Psi_2, -\underline{\bar{\Psi}})\, \Gamma(t + \Psi_2) + kV(t + \Psi_2, t + \Psi_1) - \frac{d\Psi_2}{d\tau} + \tag{2.17b}$$

$$h_2(\tau)e^{v(t + \Psi_2)}\, \Gamma(t + \Psi_2) \quad .$$

A T-periodic function $f(t)$ can be written as $\mu + \omega(t)$, where $\mu = \frac{1}{T}\int_0^T f(\zeta)d\zeta$, and $\omega(t)$ is T-periodic with zero mean. Applying this principle to (2.17a,b), we find

$$\frac{\partial \Theta_1^1}{\partial t} = \mu_1(\underline{\bar{\Psi}}) + \omega_1(t, \tau) \quad , \tag{2.18a}$$

$$\frac{\partial \Theta_2^1}{\partial t} = \mu_2(\underline{\bar{\Psi}}) + \omega_2(t, \tau) \quad . \tag{2.18b}$$

Here,

$$\mu_1 = kH(\bar{\underline{\Psi}}) + \lambda\ \beta - \frac{d\Psi_1}{d\tau} \tag{2.19a}$$

$$\mu_2 = kH(-\ \bar{\underline{\Psi}}) - \frac{d\Psi_2}{d\tau}\ , \tag{2.19b}$$

with,

$$\beta \equiv \frac{1}{T}\int_0^T \{p(\zeta)\ \Gamma(\zeta) + \gamma(\zeta)\}d\zeta\ , \tag{2.20a}$$

$$H(\bar{\underline{\Psi}}) \equiv \frac{1}{T}\int_0^T \{\rho(\zeta,\ \bar{\underline{\Psi}})\ \Gamma(\zeta) + V(\zeta,\ \zeta + \bar{\underline{\Psi}}) + r(\zeta)\}d\zeta\ . \tag{2.20b}$$

The functions $\omega_1(t,\ \tau)$ and $\omega_2(t,\ \tau)$ consist of exponentially decaying terms, and periodic terms of zero mean. Integration of (2.18) gives

$$\Theta_1^1 = \mu_1(\bar{\underline{\Psi}})t + W_1(t,\ \tau)\ , \tag{2.21a}$$

$$\Theta_2^1 = \mu_2(\bar{\underline{\Psi}})t + W_2(t,\ \tau)\ , \tag{2.21b}$$

where W_1 and W_2 are bounded functions. Substituting these values of Θ_1^1 and Θ_2^1 into (2.11c) gives

$$\frac{\partial A_2^1}{\partial t} - \Phi(t + \Psi_2)A_2^1 = \{S_1(t,\ \tau)\mu_1 + S_2(t,\ \tau)\mu_2\}t + B(t,\ \tau)\ . \tag{2.22}$$

where

$$S_1 \equiv k \frac{\partial U}{\partial \theta_1} (t + \Psi_1, t + \Psi_2) \quad ,$$

$$S_2 \equiv k \frac{\partial U}{\partial \theta_2} (t + \Psi_2, t + \Psi_1) + k\rho(t + \Psi_2, -\bar{\Psi})\, \Phi'(t + \Psi_2) \quad , \tag{2.23}$$

and $B(t, \tau)$ is a bounded function composed of T-periodic and exponentially decaying terms. For a physically meaningful solution, the amplitude correction A_2^1 and its time derivative $\frac{\partial A_2^1}{\partial t}$ must be bounded for all t. Hence, (2.22) implies

$$\{S_1(t, \tau)\mu_1 + S_2(t, \tau)\mu_2\}t \tag{2.24}$$

must be bounded for all t. S_1 and S_2 are T-periodic in t. Hence, (2.24) will be bounded only if

$$S_1(t, \tau)\mu_1 + S_2(t, \tau)\mu_2 \equiv 0 \quad . \tag{2.25}$$

Generally, S_1 and S_2 are two <u>different</u> T-periodic functions. Hence, the linear combination (2.25) will be zero only if

$$\mu_1 = kH(\bar{\Psi}) + \lambda\beta - \frac{d\Psi_1}{d\tau} = 0 \quad ,$$

$$\mu_2 = kH(-\bar{\Psi}) - \frac{d\Psi_2}{d\tau} = 0 \quad , \tag{2.26}$$

or

$$\frac{d\Psi_1}{d\tau} = kH(\bar{\Psi}) + \lambda\beta \quad , \tag{2.27a}$$

$$\frac{d\Psi_1}{d\tau} = kH(-\bar{\Psi}) \quad , \tag{2.27b}$$

where $\bar{\Psi} = \Psi_2 - \Psi_1$. Combining these equations, we find a single equation for $\bar{\Psi}$.

$$\frac{d\bar{\Psi}}{d\tau} = kP(\bar{\Psi}) - \lambda\beta \quad , \tag{2.28}$$

where

$$P(\bar{\Psi}) \equiv H(-\bar{\Psi}) - H(\bar{\Psi}) \quad . \tag{2.29}$$

This is the equation that governs the evolution of the phase shift.

We discuss some properties of $P(\bar{\Psi})$ needed for analysing the time evolution of the phase shift $\bar{\Psi}$ from equation (2.28). The key features are these: $P(\bar{\Psi})$ is T-periodic, with value 0 and slope - 2 when $\bar{\Psi}$ is an integer multiple of T. Figure 6.1 illustrates the structure of $P(\bar{\Psi})$. From its definition in (2.20b), we see that $H(\bar{\Psi})$ is T-periodic. Hence, $P(\bar{\Psi}) = H(-\bar{\Psi}) - H(\bar{\Psi})$ is T-periodic. When $\bar{\Psi}$ is 0, $P(\bar{\Psi})$ has the value $H(0) - H(0) = 0$. To show $P'(0) = -2$, it is sufficient to show $H'(0) = 1$. From the definition of $H(\bar{\Psi})$ given in (2.20b), we compute

$$H'(0) = \frac{1}{T}\int_0^T \{\frac{\partial\rho}{\partial\bar{\Psi}}(\zeta, 0)\,\Gamma(\zeta) + \frac{\partial V}{\partial\theta_2}(\zeta, \zeta)\}d\zeta \tag{2.30}$$

Recall that $\rho(\zeta, \bar{\Psi})$ is the T-periodic solution of

$$\frac{\partial \rho}{\partial \zeta} - \Phi(\zeta)\rho = U(\zeta, \zeta + \bar{\Psi}) \quad . \tag{2.31}$$

Differentiating (2.31) with respect to $\bar{\Psi}$ and setting $\bar{\Psi} = 0$, we find

$$\frac{\partial}{\partial \zeta}\left(\frac{\partial \rho}{\partial \bar{\Psi}}(\zeta, 0)\right) - \Phi(\zeta)\frac{\partial \rho}{\partial \bar{\Psi}}(\zeta, 0) = \frac{\partial U}{\partial \theta_2}(\zeta, \zeta) \quad . \tag{2.32}$$

From the definition of U given in (2.3b) we compute $\frac{\partial U}{\partial \theta_2}(\zeta, \zeta) = 0$. Hence, (2.32) has no forcing term and the only periodic solution is $\frac{\partial \rho}{\partial \bar{\Psi}}(\zeta, 0) = 0$. From the definition of V given in (2.3b), we compute $\frac{\partial V}{\partial \theta_2}(\zeta, \zeta) = 1$. Substituting these values of $\frac{\partial \rho}{\partial \bar{\Psi}}(\zeta, 0)$ and $\frac{\partial V}{\partial \theta_2}(\zeta, \zeta)$ into (2.30) gives

$$H'(0) = \frac{1}{T}\int_0^T \{0 \cdot \Gamma(\zeta) + 1\}d\zeta = 1 \quad . \tag{2.33}$$

3. Coupled Chemical Oscillators

Marek and Stuchl [6] observe the interaction between two continuous stirred tank reactors, in each of which a Belusov-Zhabotinskii reaction with different parameters in taking place. The coupling of the reactors occurs via an exchange of materials through a perforated wall that seperates the reactors.

If the parameters for both reactors are nearly identical, so that their autonomous frequencies are nearly the same, then the phase difference between the oscillations of each reactor tends to a constant value as time passes. This phenomenon is called phase locking. If the parameters of the reactors are altered so that the difference of their

autonomous frequencies is sufficiently large, the phase locking cannot be maintained. Long time intervals of slow variation in the phase difference are punctuated by brief intervals of rapid fluctuations. This behavior is called rhythm splitting.

We account for these observations by studying the time evolution of the phase shift $\underline{\bar{\Psi}}(\tau)$ which is governed by

$$\frac{d\underline{\bar{\Psi}}}{d\tau} = kP(\underline{\bar{\Psi}}) - \lambda\beta \quad . \tag{3.1}$$

Phase locking occurs at $\underline{\bar{\Psi}} = \underline{\bar{\Psi}}_0$ for which the right hand side of (3.1) is zero. The stability of the zeros is easily determined. Values of $\underline{\bar{\Psi}}_0$ at which the derivative of the right hand side is negative are stable, and values of $\underline{\bar{\Psi}}_0$ at which the derivative is positive are unstable. Thus, for $\lambda = 0$ (coupled identical oscillators) we see from Figure 6.1 that $\underline{\bar{\Psi}} \equiv 0$ is a stable solution. The coupling synchronizes identical oscillators. If $\lambda \neq 0$, $\varepsilon \neq 0$, we see that $kP(\underline{\bar{\Psi}}) - \lambda\beta$ has at least two roots in $0 \leq \Psi \leq T$ if $\min P(\underline{\bar{\Psi}}) < \frac{\lambda\beta}{k} < \max P(\underline{\bar{\Psi}})$. The root $\underline{\bar{\Psi}}_0$ with negative slope is stable, and the system will evolve to stable oscillations with constant phase shift $\underline{\bar{\Psi}}_0$.

For $\min P(\underline{\bar{\Psi}}) < \frac{\lambda\beta}{k} < \max P(\underline{\bar{\Psi}})$, the zeros of $k\,P(\underline{\bar{\Psi}}) - \lambda\beta$ depend continuously on $\frac{\lambda\beta}{k}$. At $\frac{\lambda\beta}{k} = \min_{(\max)} P(\underline{\bar{\Psi}}) = P(\underline{\bar{\Psi}}_m)$, an interesting bifurcation takes place; namely, the change from phase locking to rhythm splitting. To show this, we write (3.1) as

$$\frac{d\bar{\Psi}}{d\tau} = kP(\bar{\Psi}) - kP(\bar{\Psi}_m) + kP(\bar{\Psi}_m) - \lambda\beta = k\{P(\bar{\Psi}) - P(\bar{\Psi}_m)\} + \delta^2 , \quad (3.2)$$

where $\delta^2 = kP(\bar{\Psi}_0) - \lambda\beta$, and $\frac{\lambda\beta}{k}$ is slightly less than $\min P(\bar{\Psi}) = P(\bar{\Psi}_m)$, so that $0 < \delta << 1$. Figure 6.2 illustrates the situation with a graph of $k\{P(\bar{\Psi}) - P(\bar{\Psi}_0)\} + \delta^2$ vs. $\bar{\Psi}$. (3.2) is a singularly perturbed problem in the small parameter δ. The analysis is straightforward, we omit the details and present the results. The solution is nearly constant at the values $\bar{\Psi} = \bar{\Psi}_m + nT$, n = integer, where the right hand side is $O(1)$. Away from $\bar{\Psi} = \bar{\Psi}_m + nT$, the right hand side is $O(1)$. These regions of rapid variation in $\bar{\Psi}(\tau)$ correspond to boundary layers that join the constant values $\bar{\Psi} = \bar{\Psi}_m + nT$, as shown in Figure 6.3. This is the behavior of the phase shift $\bar{\Psi}(\tau)$ that corresponds to rhythm splitting. Once $\bar{\Psi}$ is known, we find Ψ_1 and Ψ_2 from equation (2.27). The solutions for x_i, y_i, $i = 1, 2$ are then given by

$$x_i = X(t + \Psi_i) , \; y_i = Y(t + \Psi_i) , \; i = 1,2 \quad . \quad (3.3)$$

The frequency of the oscillations in x_2 is

$$\nu = \frac{d}{dt}(t + \Psi_2) = 1 + \varepsilon \, kH(-\bar{\Psi}) \quad . \quad (3.4)$$

Figure 6.4 shows a graph of ν vs. t and Figure 6.5 shows the behavior of the concentration $x_2(t)$. The peaks in Figure 6.4 correspond to the regions of rapid change in $\bar{\Psi}(\tau)$.

CHAPTER 7

LARGE POPULATIONS OF COUPLED CHEMICAL OSCILLATORS

1. Introduction

We study the phenomenon of synchronization in large systems of chemical oscillators. By synchronization, we mean the evolution from an initial state where the phases of the oscillators are distributed randomly to a final state in which the oscillators are all in phase. The model is a direct generalization of the one used to study Marek and Stuchl's two oscillator system in Chapter 6. The model equations are

$$\begin{aligned} \dot{x}_i &= F(x_i, y_i) + \varepsilon \sum_{\ell} k(d_{i\ell}) x_\ell \quad , \\ \dot{y}_i &= G(x_i, y_i) + \varepsilon \sum_{\ell} k(d_{i\ell}) y_\ell \quad , \end{aligned} \tag{1.1}$$

where $0 < \varepsilon << 1$, and $d_{i\ell}$ is the spatial displacement between the ith and ℓth oscillators. When $\varepsilon = 0$, each (x_i, y_i) satisfies the equations

$$\dot{x} = F(x, y) \ , \ \dot{y} = G(x, y) \quad . \tag{1.2}$$

We assume that all solutions of (1.2) tend to a T-periodic limit cycle as $t \to \infty$. The limit cycle solution is denoted by

$$x = X(t + \Psi) \ , \ y = Y(t + \Psi) \quad , \tag{1.3}$$

where Ψ is an arbitrary phase shift. When $\varepsilon \neq 0$, the oscillators are

coupled. The terms $\varepsilon K(d_{\sim i\ell})x_\ell$ and $\varepsilon K(d_{\sim i\ell})y_\ell$ in the right hand side of (1.1) represent the coupling between the ith and ℓth oscillator. We assume that the coupling function $K(d_{\sim i\ell})$ goes to zero as the spatial displacement $d_{\sim i\ell}$ between the oscillators becomes infinite.

A complete solution of the discrete system (1.1), even if it were possible, would contain a lot of irrelevant information. We do not seek the detailed trajectory of each (x_i, y_i), but only the overall distribution of the oscillator's phases ψ_i as a function of time. In Section 2, we use a continuum approximation to derive an integro-differential equation that describes the time evolution of the phase distribution.

This integro-differential equation is too complex to be solved in full generality. To make further progress, one requires some simplifying assumptions. These assumptions and their consequences are pursued in Section 3.

The model (1.1) describes a variety of situations, depending on the choice of the coupling function $K(d)$. In Section 4, we study synchronization in systems where $K(p - q)$ has the same constant value for all p, q in the volume that contains the oscillators. This would represent a system of oscillators in a well stirred bath. In Section 5, we determine the $K(d)$ that corresponds to diffusive coupling of the oscillators. In Section 6, we study how autosynchronization proceeds in the case of diffusively coupled oscillators. The analysis leads to a certain singular boundary value problem. In Section 7, we perform a constructive proof for its solvability.

2. The Distribution of Phases

The asymptotic method used to study Marek and Stuchl's two

oscillator system in Chapter 6 can be applied directly to (1.1). One finds that to leading order,

$$x_i = X(t + \Psi_i(\tau)) \ , \ y_i = Y(t + \Psi_i(\tau)) \quad , \tag{2.1}$$

where $\tau = \varepsilon t$ and the phases Ψ_i obey

$$\frac{d\Psi_i}{d\tau} = \sum_{\ell} K(d_{\underset{\sim}{i\ell}}) \ P(\Psi_\ell - \Psi_i) \quad . \tag{2.2}$$

P is a T-periodic function determined from X and Y which satisfies $P'(0) = 1$. In the limit where there are many oscillators per unit volume, we can derive an equation for the distribution of phases Ψ_i.

Let $n(\Psi, \underset{\sim}{q}, \tau)d\Psi d\underset{\sim}{q}^3$ be the number of oscillators in a volume element $d\underset{\sim}{q}^3$ about spatial position $\underset{\sim}{q}$ and with phases Ψ in the interval $\left[\Psi, \Psi + d\Psi\right]$. Since oscillators are conserved, this distribution $n(\Psi, \underset{\sim}{q}, \tau)$ of points $(\Psi_i, \underset{\sim}{q}_i)$ in $(\Psi, \underset{\sim}{q})$ space must obey an equation of continuity

$$\frac{\partial n}{\partial t} + \operatorname{div}(n\underset{\sim}{U}) = 0 \quad , \tag{2.3}$$

where $\underset{\sim}{U}$ is the velocity of the flow in $(\Psi, \underset{\sim}{q})$ space. To find the Ψ component of $\underset{\sim}{U}$, we note from (2.2) that an oscillator with $\Psi_i = \Psi$ and $q_i = q$ has

$$\frac{d\Psi_i}{d\tau} = \sum_{\ell} K(\underset{\sim}{q}_\ell - \underset{\sim}{q}) \ P(\Psi_\ell - \Psi) \quad . \tag{2.4}$$

In the continuum limit, we can approximate the right hand side of (2.4) by

$$R(\Psi, \underset{\sim}{q}, \tau) \equiv \int\int_{-\pi}^{\pi} K(\underset{\sim}{p} - \underset{\sim}{q})\, P(\varphi - \Psi)\, n(\varphi, \underset{\sim}{p}, \tau) d\varphi d\underset{\sim}{p}^{3} \quad . \tag{2.5}$$

This gives the Ψ component of $\underset{\sim}{U}$. The $\underset{\sim}{q}$ component is assumed to be zero, corresponding to a system of oscillators whose positions are fixed. With $\underset{\sim}{U}$ given by

$$\underset{\sim}{U} = (R(\Psi, \underset{\sim}{q}, \tau) \ , \ 0) \quad , \tag{2.6}$$

(2.3) becomes

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial \Psi} (nR) = 0 \quad , \tag{2.7}$$

where R is given by (2.5). From the form of R, we see that (2.7) is a nonlinear integro-differential equation for the distribution of phases $n(\Psi, \underset{\sim}{q}, \tau)$. This equation can be cast in an alternative form. Writing (2.7) as

$$\frac{\partial n}{\partial t} + R \frac{\partial n}{\partial \Psi} = - n \frac{\partial R}{\partial \Psi} \quad , \tag{2.8}$$

we see that it admits the characteristic form

$$\frac{dn}{d\tau} = - n \frac{\partial R}{\partial \Psi} \text{ along } \frac{d\Psi}{d\tau} = R \quad . \tag{2.9a,b}$$

3. A Special Class of Solutions

The integro-differential equation for $n(\Psi, \underset{\sim}{q}, \tau)$ is too complex to be solved in full generality. To make further progress, we introduce some simplifying assumptions. Since we don't expect the process of synchronization to depend strongly on the detailed form of the limit cycle given in (1.3), we assume a circular limit cycle, with

$$x = \cos(t + \Psi) \ , \ y = \sin(t + \Psi) \quad . \tag{3.1}$$

In this case, the periodic function $P(\Theta)$ which appears in (2.5) is given by

$$P(\Theta) = \sin \Theta \quad . \tag{3.2}$$

With this form of $P(\Theta)$, the function $R(\Psi, \underset{\sim}{q}, \tau)$ given in (2.5) can be written as

$$R(\Psi, \underset{\sim}{q}, \tau) = \alpha(\underset{\sim}{q}, \tau) \cos \Psi + \beta(\underset{\sim}{q}, \tau) \sin \Psi \quad , \tag{3.3}$$

where

$$\alpha(\underset{\sim}{q}, \tau) \equiv \int\int_{-\pi}^{\pi} K(\underset{\sim}{p} - \underset{\sim}{q}) \sin \varphi \, n(\varphi, \underset{\sim}{p}, \tau) d \, dp^3 \quad , \tag{3.4}$$

$$\beta(\underset{\sim}{q}, \tau) \equiv - \int\int_{-\pi}^{\pi} K(\underset{\sim}{p} - \underset{\sim}{q}) \cos \varphi \, n(\varphi, \underset{\sim}{p}, \tau) d \, dp^3 \quad . \tag{3.5}$$

Hence, the equation for the characteristics (2.9b) reads

$$\frac{d\Psi}{d\tau} = \alpha(\underset{\sim}{q}, \tau) \cos \Psi + \beta(\underset{\sim}{q}, \tau) \sin \Psi \quad . \tag{3.6}$$

A further simplification is possible. If we seek solutions $n(\Psi, \underset{\sim}{q}, \tau)$ that are even in Ψ, then it follows from (3.4) that $\alpha(\underset{\sim}{q}, \tau) \equiv 0$, and (3.6) reduces to

$$\frac{d\Psi}{d\tau} = \beta(\underset{\sim}{q}, \tau) \sin \Psi \quad . \tag{3.7}$$

(3.7) can be integrated to yield

$$\tan \frac{\Psi}{2} = e^{B(\underset{\sim}{q}, \tau)} \tan \frac{\Psi_o}{2} \quad , \tag{3.8}$$

where Ψ_o is the value of Ψ at $\tau = 0$ and

$$B(\underset{\sim}{q}, \tau) = \int_o^\tau \beta(\underset{\sim}{q}, u)du \quad . \tag{3.9}$$

For fixed $\underset{\sim}{q}$, (3.8) gives the characteristics in the Ψ, τ plane. We note that the plot of the characteristics in the (Ψ, τ) plane is symmetric about the line $\Psi = 0$ as shown in Figure 7.1. Hence, if $n(\Psi, \underset{\sim}{q}, \tau)$ is initially even in Ψ, it remains even in Ψ.

The function $B(\underset{\sim}{q}, \tau)$ is the key to understanding the synchronization process. If $B(\underset{\sim}{q}, \tau) \to -\infty$ as $\tau \to \infty$, then we find from (3.8) that characteristics $\Psi(\tau)$ with $-\pi < \Psi(0) < \pi$ all converge to $\Psi = 0$ as $\tau \to \infty$. The phases of the oscillators all synchronize to the value 0.

If $B(\underset{\sim}{q}, \tau) \to +\infty$ as $\tau \to \infty$, then the phases of the oscillators synchronize to $\Psi = -\pi$ or $\Psi = +\pi$. In this latter case, we note that $-\pi$ and $+\pi$ are physically indistinguishable, both corresponding to the same point in the cycle of an oscillation.

We seek a governing equation for $B(\underset{\sim}{q}, \tau)$. The first step is to compute the density $n(\Psi, \underset{\sim}{q}, \tau)$ from initial values $n(\Psi, \underset{\sim}{q}, 0) = n_o(\Psi, \underset{\sim}{q})$. Referring to Figure 7.2 we see the basic idea of this calculation. Phases Ψ_i in the interval $\left[\Psi_o, \Psi_o + d\Psi_o\right]$ are transported via the characteristics to the interval $\left[\Psi, \Psi + d\Psi\right]$ in time τ. Hence, the density at $(\Psi, \underset{\sim}{q}, \tau)$ is related to the initial value at $(\Psi_o, \underset{\sim}{q}, \tau)$ via

$$n(\Psi, \underset{\sim}{q}, \tau)d\Psi = n_o(\Psi_o, \underset{\sim}{q})d\Psi_o \quad . \tag{3.10}$$

Using the expression (3.8) for the characteristics, a simple calculation yields

$$n(\Psi, \underset{\sim}{q}, \tau) = \nu(\Psi, \underset{\sim}{q}, B(\underset{\sim}{q}, \tau)) \quad . \tag{3.11}$$

where

$$\nu(\Psi, \underset{\sim}{q}, \tau) \equiv \frac{n_o(2 \arctan (e^{-B} \tan \frac{\Psi}{2}), \underset{\sim}{q})}{\cosh B + \sinh B \cos \Psi} \quad . \tag{3.12}$$

The final step to finding the equation for $B(\underset{\sim}{q}, \tau)$ is to recall the definition

$$\beta \equiv -\int\int_{-\pi}^{\pi} K(\underset{\sim}{p} - \underset{\sim}{q}) \cos \varphi \; n(\varphi, \underset{\sim}{p}, \tau) d\varphi d\underset{\sim}{p}^3 \quad . \tag{3.13}$$

From (3.9), we have $\beta = \frac{\partial B}{\partial \tau}$ and from (3.11) we have $n(\varphi, \underset{\sim}{p}, \tau) = \nu(\varphi, \underset{\sim}{p}, B(\underset{\sim}{p}, \tau))$. Substituting these values of β and n into (3.13) gives

$$\frac{\partial B}{\partial \tau} = - \int\int_{-\pi}^{\pi} K(\underset{\sim}{p} - \underset{\sim}{q}) \cos\varphi \; \nu(\varphi, \underset{\sim}{p}, B(\underset{\sim}{p}, \tau)) d\varphi d\underset{\sim}{p}^3 \quad . \tag{3.14}$$

This is an integro-differential equation for B. From (3.9), we see that the initial condition is $B(q, 0) = 0$. In its full generality, this problem is still very formidable. To make further progress, we restrict our attention to an important special case.

We study the process of synchronization in a system where a certain fraction of the oscillators are initially synchronized, while the remainder have a random distribution of phases. The initial distribution of phases is

$$n_o(\Psi, \underset{\sim}{q}) = \frac{\rho(\underset{\sim}{q})}{2\pi} + u(\underset{\sim}{q}) \; \delta(\Psi) \quad . \tag{3.15}$$

The first term $\frac{\rho(\underset{\sim}{q})}{2\pi}$ represents the random component, while the delta function $u(\underset{\sim}{q}) \; \delta(\Psi)$ represents the synchronized component. With n_o so chosen, we determine the corresponding value of $\nu(\Psi, \underset{\sim}{q}, B)$ from (3.12) and substitute it into the integral equation (3.13). With the special value of $\nu(\varphi, \underset{\sim}{q}, B)$, one finds that the integration over phases φ can be done explicitly. The result of the calculation is

$$\frac{\partial B}{\partial \tau} = \int K(\underset{\sim}{p} - \underset{\sim}{q}) \; \{\rho(\underset{\sim}{p}) \tanh \frac{B}{2} - u(\underset{\sim}{p})\} d\underset{\sim}{p}^3 \quad . \tag{3.16}$$

Our aim is to study this equation for various choices of the coupling function $K(\underset{\sim}{d})$. Once $B(\underset{\sim}{q}, \tau)$ is known, the characteristics are given by (3.7) and the density $n(\Psi, \underset{\sim}{q}, \tau)$ by (3.13) and (3.14).

4. Oscillators in a Well Stirred Bath

We study the process of synchronization in a system where the coupling between any two oscillators is independent of their positions. Hence, we take $K(\underset{\sim}{p} - \underset{\sim}{q}) \equiv 1$ for all $\underset{\sim}{p}$ and $\underset{\sim}{q}$ inside the volume that contains the oscillators. Since spatial position is now irrelevant in the synchronizing process, we take ρ, u and $n = n(\Psi, \tau)$ independent of position $\underset{\sim}{q}$. In the initial condition (3.16), we take $\rho >> u$, so that initially, the random component dominates the synchronized component. With these simplifications, (3.18) becomes a first order ODE,

$$\frac{dB}{d\tau} = N \tanh \frac{B}{2} - uV \quad , \tag{4.1}$$

where N is the total number of oscillators and V is the volume of the system. The initial condition is $B(0) = 0$.

Suppose $u = 0$, corresponding to a completely random initial distribution of phases. Then the solution of (4.1) is $B \equiv 0$, and it follows from (3.7) that the characteristics of the Ψ,τ plane are vertical straight lines. The initial random distribution of phases persists for all time. We can understand this result by inspecting the coupling terms of (1.1). In the present case,

$$\varepsilon \sum_{\ell} K(d_{i\ell}) \, x_{\ell}(t) \sim \varepsilon \sum_{\ell} \cos(t + \Psi_{\ell})$$
$$\varepsilon \sum_{\ell} K(d_{i\ell}) \, y_{\ell}(t) \sim \varepsilon \sum_{\ell} \sin(t + \Psi_{\ell}) \quad . \tag{4.2}$$

If the phases Ψ_{ℓ} vary randomly over $(-\pi, \pi)$ then the different signals $\varepsilon \cos(t + \Psi_{\ell})$ and $\varepsilon \sin(t + \Psi_{\ell})$ interfere destructively, and the coupling terms are nearly zero. There is no forcing to initiate synchronization.

This steady state solution is unstable. Figure 7.3 shows a graph of $\frac{dB}{d\tau}$ vs B for $0 < u << 1$. The arrows along the $-B$ axis indicate the motion of $B(\tau)$, starting from $B = 0$. Notice that the effect of the $O(u)$ term in (4.1) is to give $B(\tau)$ a small initial boost away from $B = 0$. When B becomes larger than $O(u)$, the motion is governed to leading order by

$$\frac{dB}{d\tau} = N \tanh \frac{B}{2} \quad . \tag{4.3}$$

The solution with B tending to $-\infty$ has

$$B \to -N\tau + \text{const.} \text{ as } \tau \to \infty \quad . \tag{4.4}$$

Hence, the equation for the characteristics (3.8) becomes

$$\tan \frac{\Psi}{2} = C \, e^{-N\tau} \tan \frac{\Psi_o}{2} \text{ as } \tau \to \infty \quad . \tag{4.5}$$

The characteristics are plotted in Figure 7.4. Notice that they all

converge to $\Psi = 0$. We are witnessing the evolution of the system from an initial state with a nearly uniform distribution of phases to a final state in which all the oscillators are synchronized, with $\Psi = 0$. Figure 7.5 shows graphs of the density n corresponding to the initial and final states.

5. A Model of Diffusive Coupling

We perform a simple analysis to determine the form of coupling function $K(\underset{\sim}{d})$ that corresponds to diffusion. Suppose the oscillators are distributed uniformly in space, and that an oscillator at spatial position $\underset{\sim}{q}$ has $x_i = x(\underset{\sim}{q}, t)$ and $y = y(\underset{\sim}{q}, t)$. In this case, we replace (1.1) by the continuum approximation

$$\begin{aligned} \frac{\partial x}{\partial t} &= F(x, y) + \varepsilon \int K(\underset{\sim}{p} - \underset{\sim}{q})\, x(\underset{\sim}{p}, t)\, d\underset{\sim}{p}^3 \quad , \\ \frac{\partial y}{\partial t} &= G(x, y) + \varepsilon \int K(\underset{\sim}{p} - \underset{\sim}{q})\, y(\underset{\sim}{p}, t)\, d\underset{\sim}{p}^3 \quad . \end{aligned} \tag{5.1}$$

If $K(\underset{\sim}{p}) = \nabla^2\, \delta(\underset{\sim}{p})$, then (5.1) becomes

$$\begin{aligned} \frac{\partial x}{\partial t} &= F(x, y) + \varepsilon\, \nabla^2\, x \\ \frac{\partial y}{\partial t} &= G(x, y) + \varepsilon\, \nabla^2\, y \quad . \end{aligned} \tag{5.2}$$

This is the reaction diffusion system studied in Chapter 5. Hence $K(\underset{\sim}{d}) = \nabla^2\, \delta(\underset{\sim}{d})$ provides a model of diffusive coupling.

6. A Diffusively Coupled System

We study synchronization in a system of diffusively coupled oscillators. Initially, the phases Ψ of the oscillators are distributed uniformly throughout $[-\pi, \pi]$, except for those oscillators in an infinitesimal neighborhood of spatial position $\underset{\sim}{q} = 0$, which are constrained to have $\Psi = 0$ for all slow time $\tau > 0$. That is,

$$n(\Psi, \underset{\sim}{q}, \tau) \to \delta(\Psi) \tag{6.1}$$

as $\underset{\sim}{q} \to \underset{\sim}{0}$ for fixed $\tau > 0$. While

$$n(\Psi, \underset{\sim}{q}, 0) = n_o(\Psi, \underset{\sim}{q}) = \frac{1}{2\pi} \tag{6.2}$$

for $\underset{\sim}{q} \neq \underset{\sim}{0}$. The oscillators at $\underset{\sim}{q} = 0$ can be regarded as pacemakers that initiate a synchronization process in the rest of the medium.

To see how this synchronization process proceeds, we must determine the solution for $B(\underset{\sim}{q}, \tau)$. Comparing (6.2) with the initial condition (3.16), we find that

$$\rho(\underset{\sim}{q}) = 1 \ , \ u(\underset{\sim}{q}) = 0 \tag{6.3}$$

for $\underset{\sim}{q} \neq 0$. With these values for ρ and u, and $K(\underset{\sim}{q}) = \nabla^2 \delta(\underset{\sim}{q})$, the equation (3.15) for $B(\underset{\sim}{q}, \tau)$ reads

$$\frac{\partial B}{\partial \tau} = \nabla^2 \left(\tanh \frac{B}{2}\right) \ . \tag{6.4}$$

The initial condition is $B(\underset{\sim}{q}, 0) = 0$ for $\underset{\sim}{q} \neq 0$. To determine the condition on B at $\underset{\sim}{q} = 0$, we recall that the distribution of phases becomes sharply peaked about $\Psi = 0$ as B becomes large and negative. Since $n(\Psi, \underset{\sim}{q}, \tau) = \delta(\Psi)$ as $\underset{\sim}{q} \to 0$, we require $B(\underset{\sim}{q}, \tau) \to -\infty$ as $\underset{\sim}{q} \to 0$ for fixed $\tau > 0$.

It is convenient to introduce the variable $U = \tanh \frac{B}{2}$. The problem for U is

$$\frac{\partial U}{\partial \tau} = \tfrac{1}{2}(1 - U^2)\, \nabla^2 U \ , \ \tau > 0 \tag{6.5}$$

$$U(\underset{\sim}{q}, 0) = 0 \ , \ U(\underset{\sim}{0}, \tau) = -1 \text{ for } \tau > 0 \ . \tag{6.6}$$

We consider the one dimensional case, with $\underset{\sim}{q}$ replaced by a scalar q and ∇^2 replaced by $\frac{\partial^2}{\partial q^2}$. This one dimensional problem admits a similarity solution $U = X(s)$, where $s = \frac{|q|}{\sqrt{\tau}}$ and $X(s)$ satisfies

$$X'' = -\frac{s}{1 - X^2} X' \text{ on } 0 \underset{\neq}{<} x \underset{=}{<} \infty \ , \tag{6.7}$$

$$X(0) = -1 \ , \ X(\infty) = 0 \ . \tag{6.8}$$

In Section 7, we prove that this singular boundary value problem has a monotone increasing solution $X(s)$.

With this solution for $X(s)$ one can determine $B(q, \tau)$ from

$$B(q, \tau) = \tfrac{1}{2} \log \frac{1+X\left(\frac{|q|}{\sqrt{\tau}}\right)}{1-X\left(\frac{|q|}{\sqrt{\tau}}\right)} \quad . \tag{6.9}$$

As $\tau \to +\infty$ with q fixed, $X\left(\frac{|q|}{\sqrt{\tau}}\right) \to -1$ and $B \to -\infty$. Hence, for each q, the picture of the characteristics in the (Ψ, τ) plane looks like Figure 7.4 with all the characteristics converging to $\Psi = 0$. The rate of synchronization is determined by q, decreasing as $|q| \to \infty$. This is illustrated in Figure 7.6, where $n(\Psi, q, \tau)$ is plotted vs. Ψ for various q at a fixed instant of time τ.

7. An Existence Theorem

We prove that the singular boundary value problem

$$\begin{aligned} X'' &= -\frac{s}{1-X^2} X' \text{ on } 0 \leq s < \infty \quad , \\ X(0) &= -1 \ , \ X(\infty) = 0 \quad , \end{aligned} \tag{7.1}$$

has a monotone increasing solution. The proof employs an iteration scheme on an equivalent integral equation. This scheme is an alternating pincer movement, analogous to the one employed in D.S. Cohen's treatment of a nonlinear two point boundary value problem [7].

For our constructive proof, it is convenient to consider $Y = -X(s)$. We seek a monotone decreasing solution of

$$Y'' = -\frac{s}{1-Y^2} Y' \text{ on } 0 \leq s < \infty \quad , \tag{7.2}$$

It is easily verified that the iterates for $n \geq 1$ are well defined, positive, decreasing functions with $Y_n(0) = 1$, $Y_n(\infty) = 0$. Using the facts that $0 < Y_1 < 1$ and $0 < Y_2 < 1$ in $0 < s < \infty$, and the Lemma 7.1, we decue the ordering of the Y_n. The result is given in

Lemma 7.2. In $0 < s < \infty$, we have

$0 \equiv Y_0 < Y_2 \leq Y_4 \leq \ldots Y_{2n} \leq \ldots Y_{2n+1} \leq \ldots Y_3 \leq Y_1 < 1$. We see that the even iterates converge to a lower limit function $Y_L(s)$ and that the odd iterates converge to an upper limit function $Y_R(s)$. Clearly, $Y_L(s) \leq Y_R(s)$. To show that the pincer movement closes, so that the sequence Y_n converges to a solution of the boundary value problem (7.2), we prove the reverse inequality.

Theorem. $Y_R(s) \leq Y_L(s)$.

Proof. $Y_L(s)$ and $Y_R(s)$ satisfy the equations

$$Y_L(s) = F\left[Y_R\right](s) = 1 - \frac{G\left[Y_R\right](s)}{G\left[Y_R\right](\infty)} \quad . \tag{7.11}$$

$$Y_R(s) = F\left[Y_L\right](s) = 1 - \frac{G\left[Y_L\right](s)}{G\left[Y_L\right](\infty)} \quad . \tag{7.12}$$

Differentiating equations (7.11) and (7.12) with respect to s gives

$$Y_L'(s) = Y_L'(0)\, e^{-\int_0^s \frac{\nu}{1 - Y_R^2(\nu)}\, d\nu} \quad , \tag{7.13}$$

$$Y_R'(s) = Y_R'(0)\, e^{-\int_0^s \frac{\nu}{1 - Y_L^2(\nu)}\, d\nu} \quad , \tag{7.14}$$

$$Y(0) = 1 \ , \ Y(\infty) = 0 \ . \tag{7.2}$$

The boundary value problem (7.2) is equivalent to the integral equation

$$Y(s) = F\left[y\right](s) = 1 \ \frac{G\left[Y\right](s)}{G\left[Y\right](\infty)} \ , \tag{7.3}$$

where

$$G\left[Y\right](s) = \int_o^s e^{-\int_o^u \frac{\nu d\nu}{1 - Y^2(\nu)}} du \ . \tag{7.4}$$

The operator F has a property that is crucial to all our results.

Lemma 7.1. If $0 < Y_1(s) \leq Y_2(s) < 1$ for $0 < s < \infty$, then $1 > F\left[Y_1\right](s) \geq F\left[Y_2\right](s) > 0$ for $0 < s < \infty$.

Proof. We first note that $F\left[Y\right](s)$ is well defined for $Y(s)$ with $0 < Y(s) < 1$ in $0 < s < \infty$, and that $0 < F\left[Y\right](s) < 1$. These follow immediately from the definitions (7.3) and (7.4). Since the integrand in (7.4) is positive and bounded above by $e^{-\frac{u^2}{2}}$, $G\left[Y\right](\infty)$ exists, and $G\left[Y\right](s) < G\left[Y\right](\infty)$. Hence, $F\left[Y\right](s) = 1 - \frac{G\left[Y\right](s)}{G\left[Y\right](\infty)}$ has $0 < F\left[Y\right](s) < 1$ in $0 < s < \infty$.

To prove that $F\left[Y_1\right](s) \geq F\left[Y_2\right](s)$, it is sufficient to show that

$$M \equiv G\left[Y_1\right](\infty) \, G\left[Y_2\right](s) - G\left[Y_1\right](s) \, G\left[Y_2\right](\infty) \geq 0 \ . \tag{7.5}$$

Using the definition of G, (7.5) can be written as

$$M = \int_0^\infty \int_0^s \{e^{-\phi_2(u) - \phi_1(\nu)} - e^{-\phi_1(u) - \phi_2(\nu)}\} du d\nu \ , \tag{7.6}$$

where

$$\phi_k(u) = \int_0^u \frac{\nu}{1 - Y_k^2(\nu)}\, d\nu \ , \ k = 1,2 \quad . \tag{7.7}$$

The integrand of (7.6) is antisymmetric about the line $u = \nu$, hence, the contribution to the integral from the square $0 < u < s$, $0 < \nu < s$ is zero. This allows us to change the region of integration from $0 < u < s$, $0 < \nu < \infty$ to $0 < u < s < \nu < \infty$. With this change in the region of integration, and some simple algebraic manipulations, (7.6) becomes

$$M = \int_s^\infty \int_0^s e^{-\phi_1(u) - \phi_2(\nu)} \{e^{\Gamma(\nu) - \Gamma(u)} - 1\} du d\nu \ , \tag{7.8}$$

where

$$\Gamma(u) = \phi_2(u) - \phi_1(u) = \int_0^u \left\{ \frac{1}{1 - Y_2^2} - \frac{1}{1 - Y_1^2} \right\} d\nu \quad . \tag{7.9}$$

Since $0 < Y_1 \leq Y_2 < 1$ in $s > 0$, the integrand in (7.9) is non-negative. Hence, $\Gamma(u)$ is a monotone increasing function. The monotone increasing nature of $\Gamma(u)$ implies that the integrand of (7.8) is non-negative in the region of integration, which has $0 < u < s < \nu < \infty$. We conclude that $M \geq 0$.

Define the sequence $Y_n(s)$ by

$$Y_0(s) \equiv 0 \ , \ Y_{n+1}(s) = F\left[Y_n\right](s) \quad . \tag{7.10}$$

where

$$Y_L'(0) = -\frac{1}{G\left[Y_R\right](\infty)}\ ,\quad Y_R'(0) = -\frac{1}{G\left[Y_L\right](\infty)}\ . \tag{7.15}$$

Using the facts that $0 < Y_L(s) \leq Y_R(s) < 1$ in $s > 0$, and $X_L'(0) < 0$, we argue from (7.13) that

$$Y_L'(s) = Y_L'(0)\, e^{-\int_0^s \frac{\nu d\nu}{1 - Y_R^2(\nu)}} \geq Y_L'(0)\, e^{-\int_0^s \frac{\nu d\nu}{1 - Y_L^2(\nu)}} \tag{7.16}$$

From (7.14), we have

$$e^{-\int_0^s \frac{\nu d\nu}{1 - Y_L^2(\nu)}} = \frac{Y_R'(s)}{Y_R'(0)}\ . \tag{7.17}$$

Hence, (7.16) becomes

$$Y_L'(s) \geq \frac{Y_L'(0)}{Y_R'(0)}\, Y_R'(s)\ . \tag{7.18}$$

From (7.15), we see that

$$\frac{Y_L'(0)}{Y_R'(0)} = \frac{G\left[Y_R\right](\infty)}{G\left[Y_L\right](\infty)}\ . \tag{7.19}$$

From the definition (7.4) of $G\left[Y\right]$, and the fact $0 < Y_L(s) \leq Y_R(s) < 1$ in $s > 0$, we find

$$0 < G\left[Y_R\right](\infty) \leq G\left[Y_L\right](\infty)\ . \tag{7.20}$$

Hence, (7.19) implies that $0 < \frac{Y_L'(0)}{Y_R'(0)} \leq 1$ and (7.18) together with $Y_L'(s), Y_R'(s) < 0$, implies

$$Y_L'(s) \geq Y_R'(s) \quad . \tag{7.21}$$

Hence

$$Y_L(s) = 1 + \int_0^s Y_L'(\nu)d\nu \geq 1 + \int_0^s Y_R'(\nu)d\nu = Y_R(s) \quad . \tag{7.22}$$

This is the required result. The pincer movement in (7.10) closes, and the sequence $\{Y_n\}$ converges to a single limit $Y(s)$, which satisfies

$$Y(s) = F\left[Y\right](s) \quad . \tag{7.23}$$

$Y(s)$ provides the solution to the boundary value problem (7.2). Since, the iterates $Y_n(s)$ are all monotone decreasing, the solution $Y(s)$ is monotone decreasing.

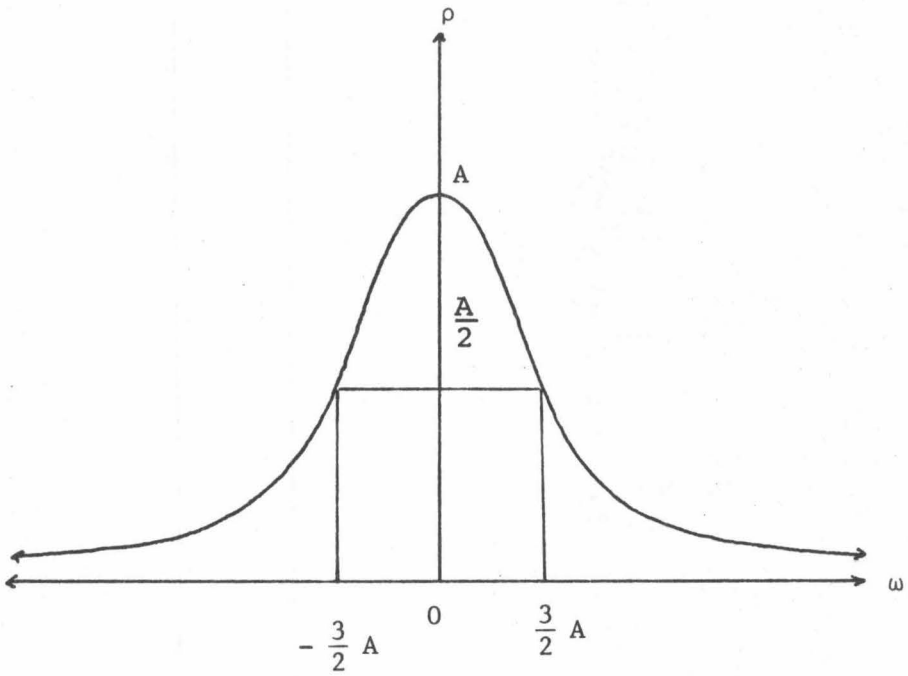


FIGURE 1.1

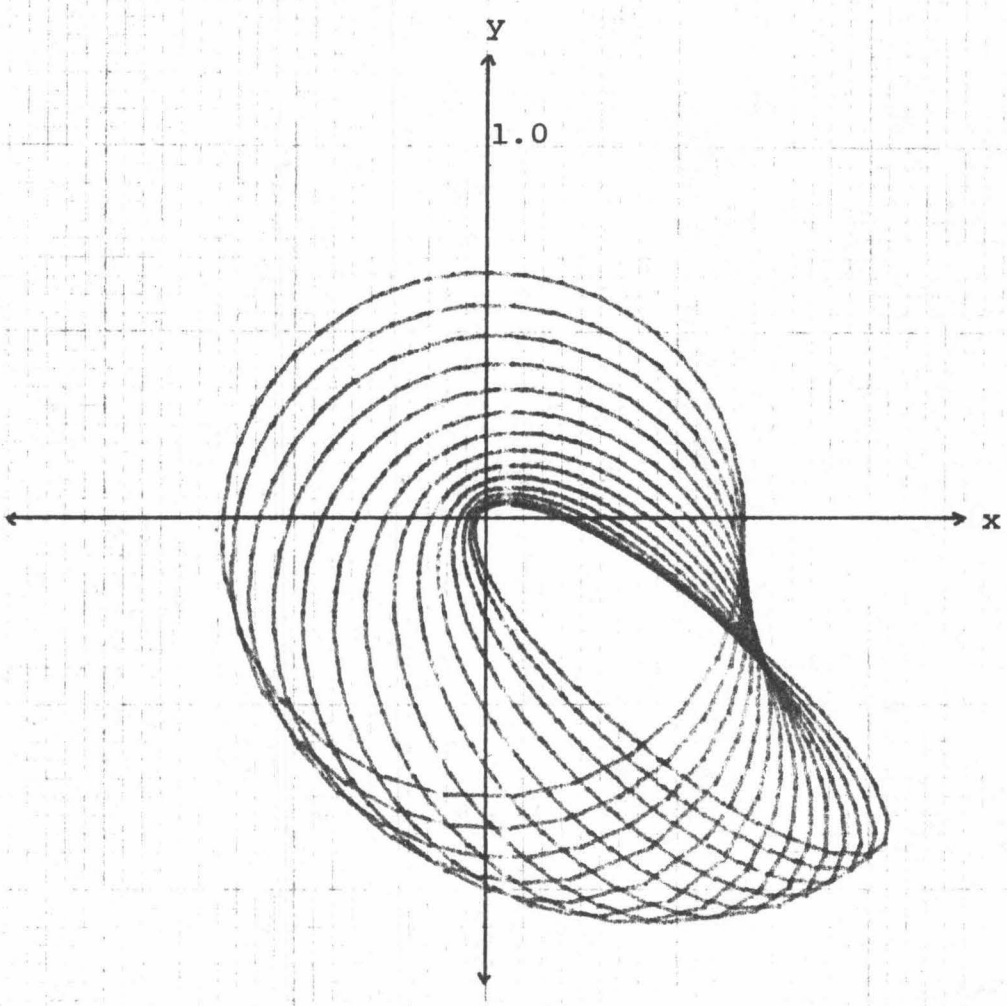
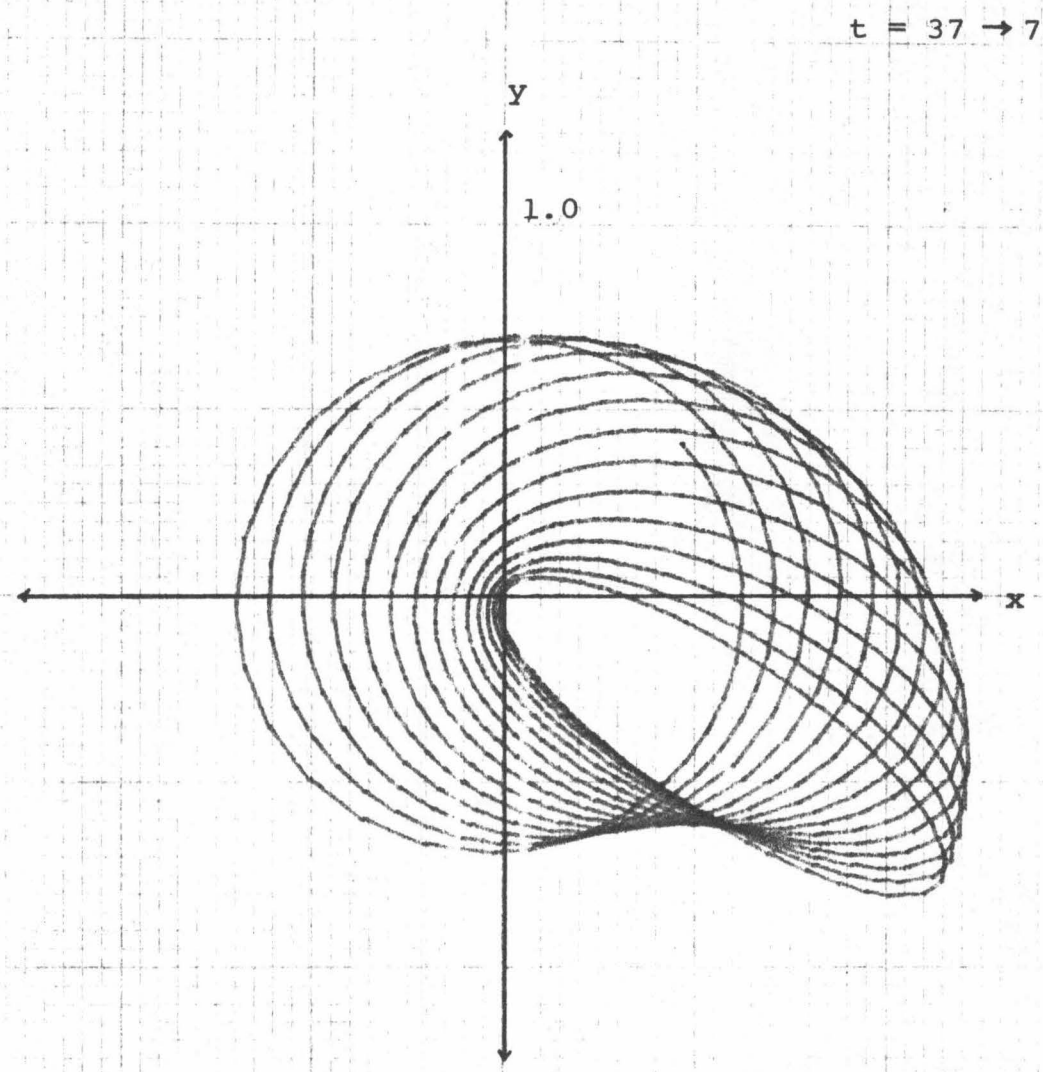


FIGURE 1.2



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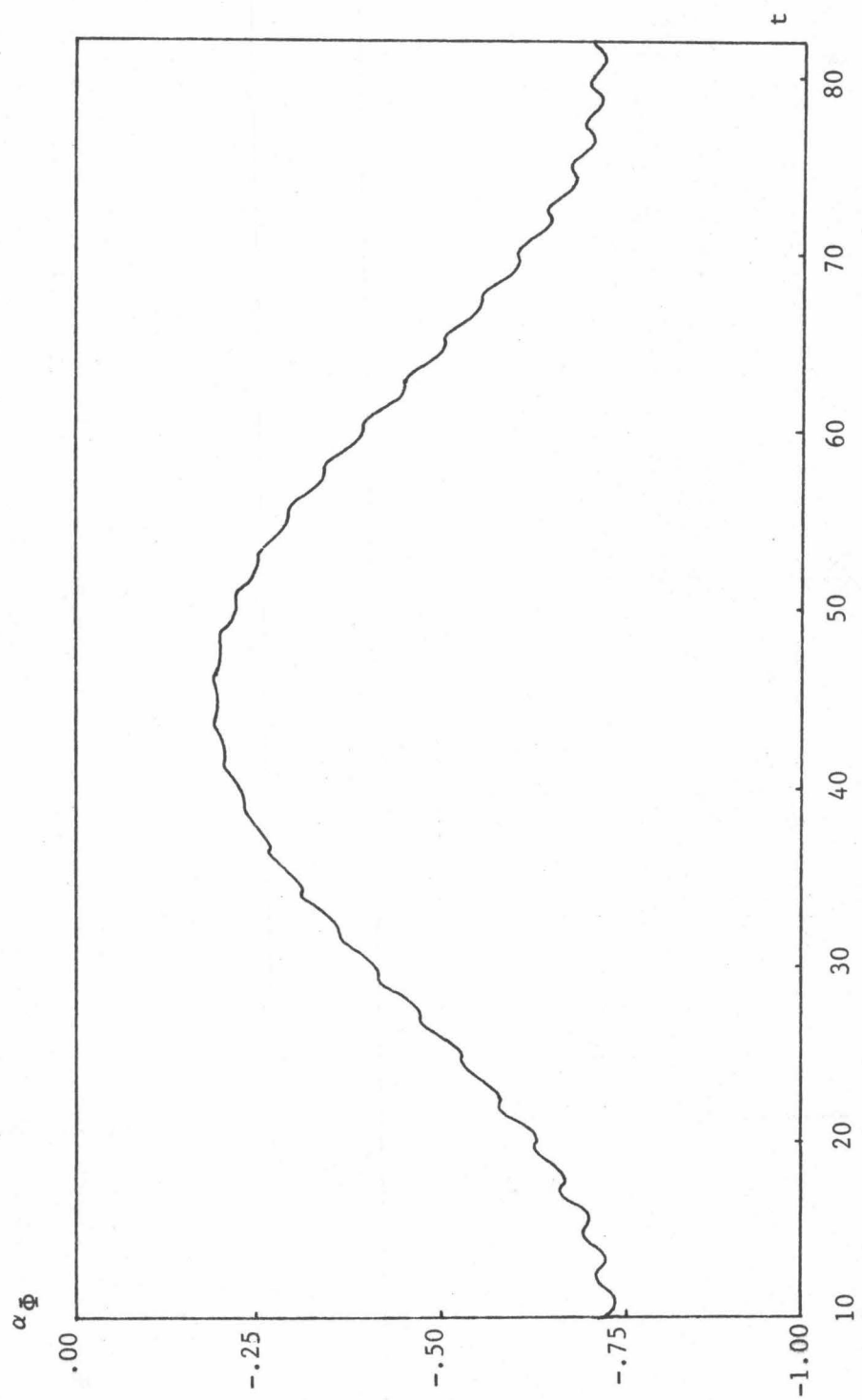


FIGURE 1.3

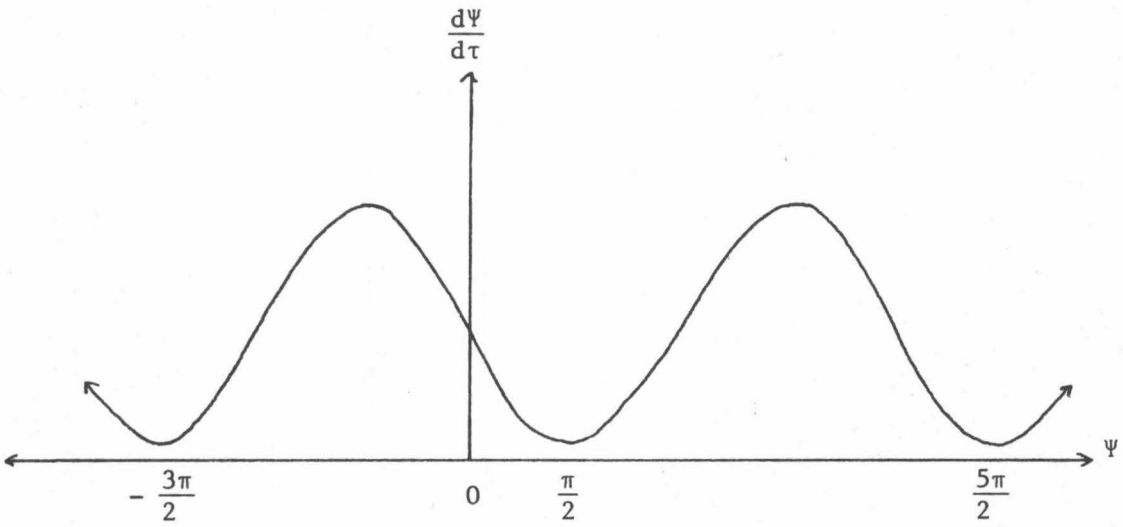


FIGURE 2.1

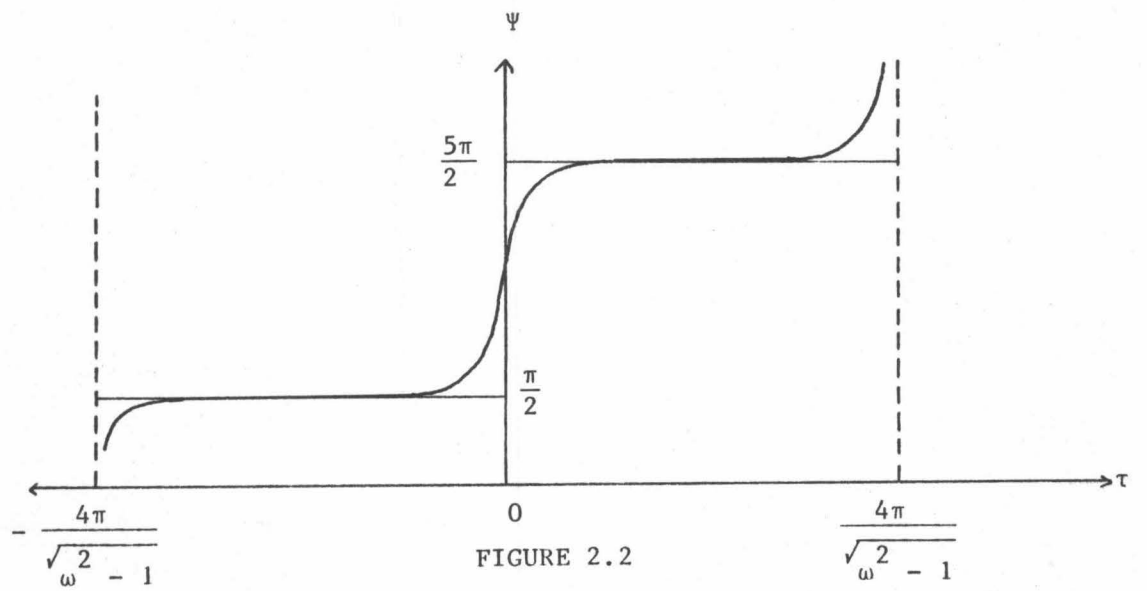
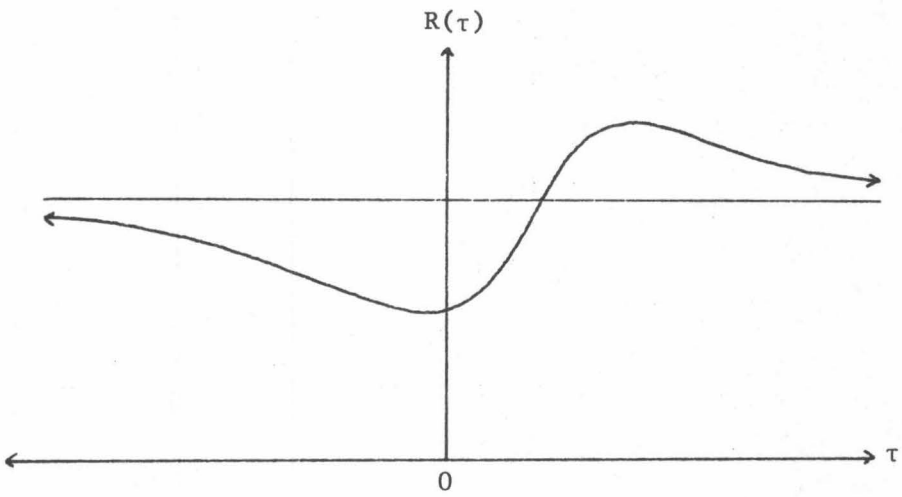


FIGURE 2.2



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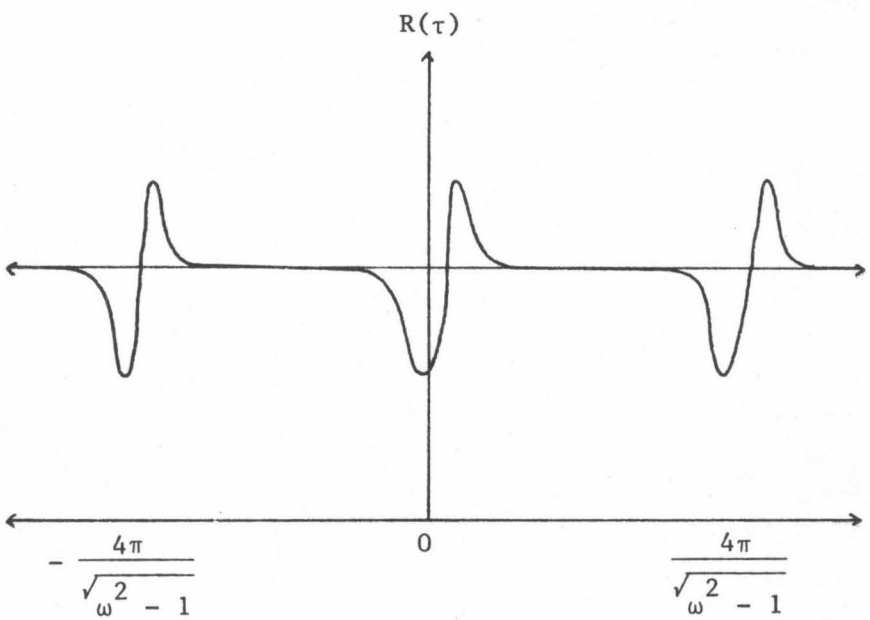


FIGURE 2.4

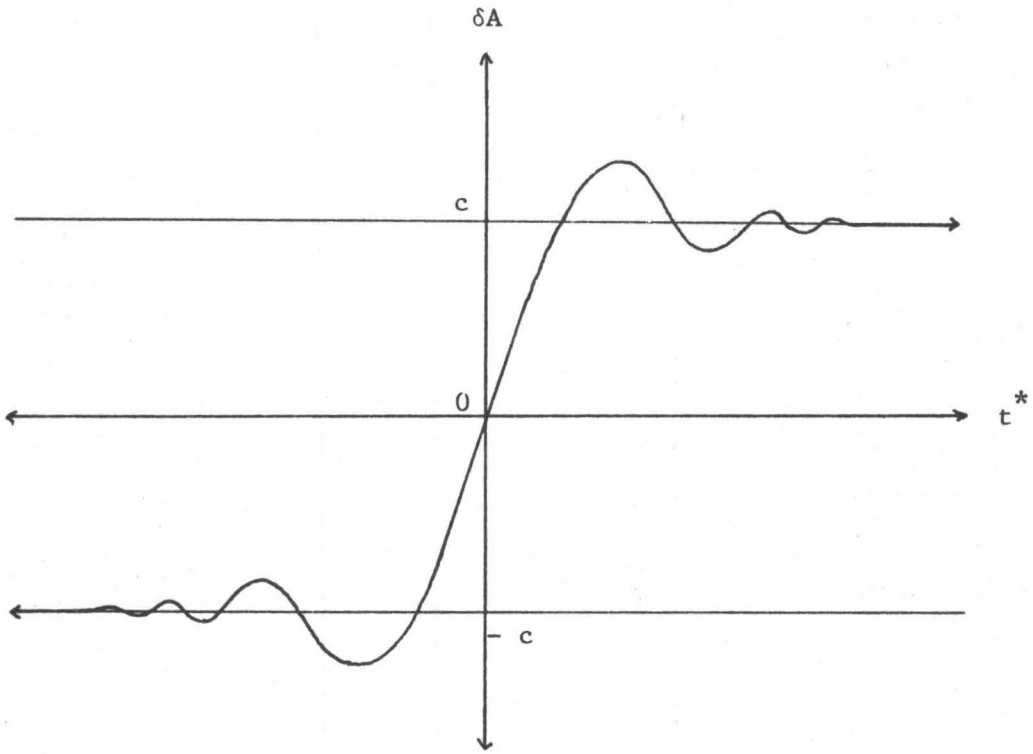


FIGURE 3

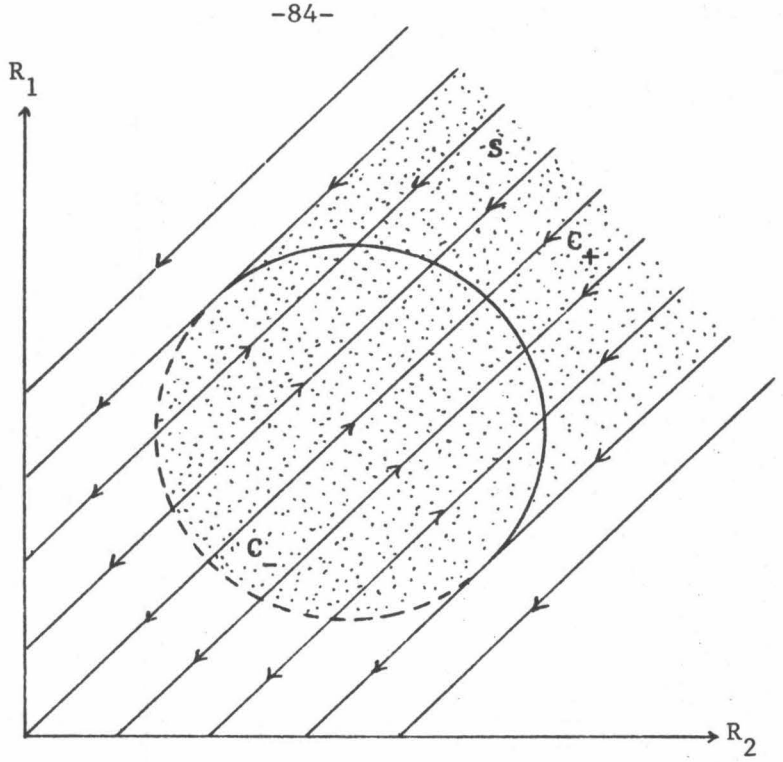


FIGURE 4.1

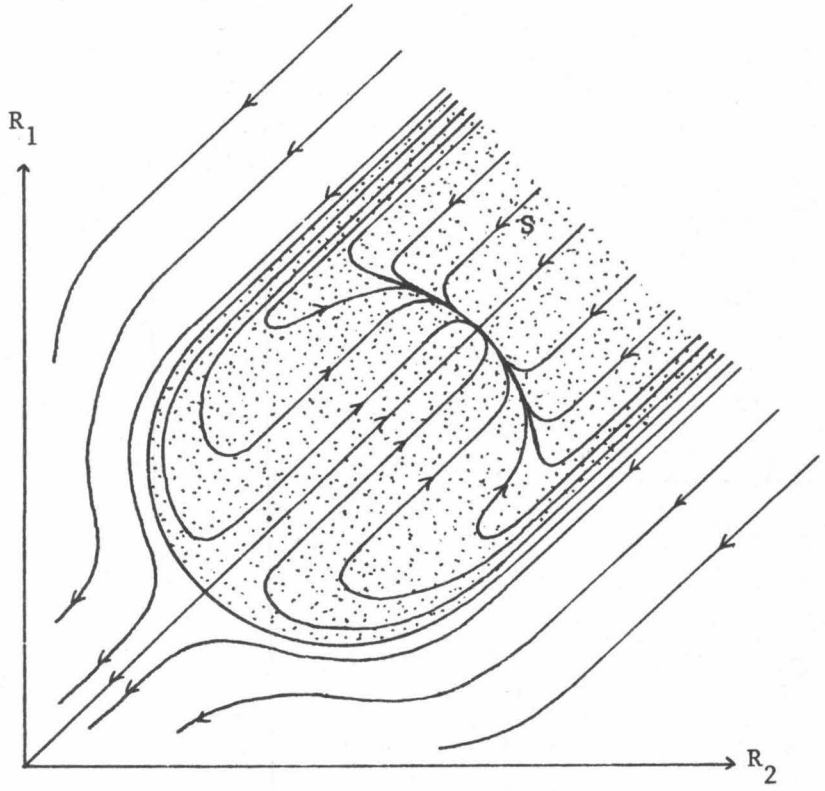


FIGURE 4.2

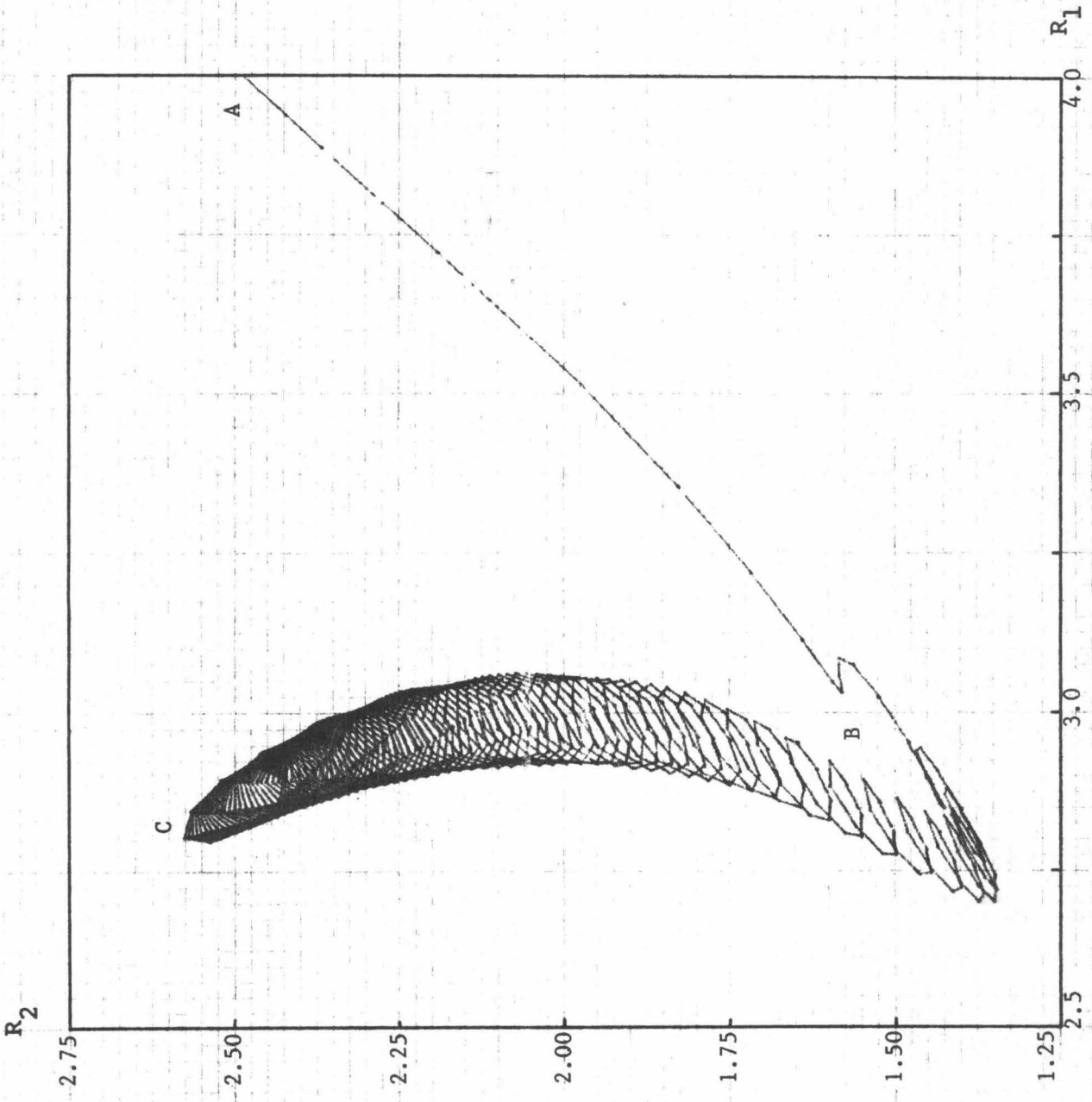


FIGURE 4.3

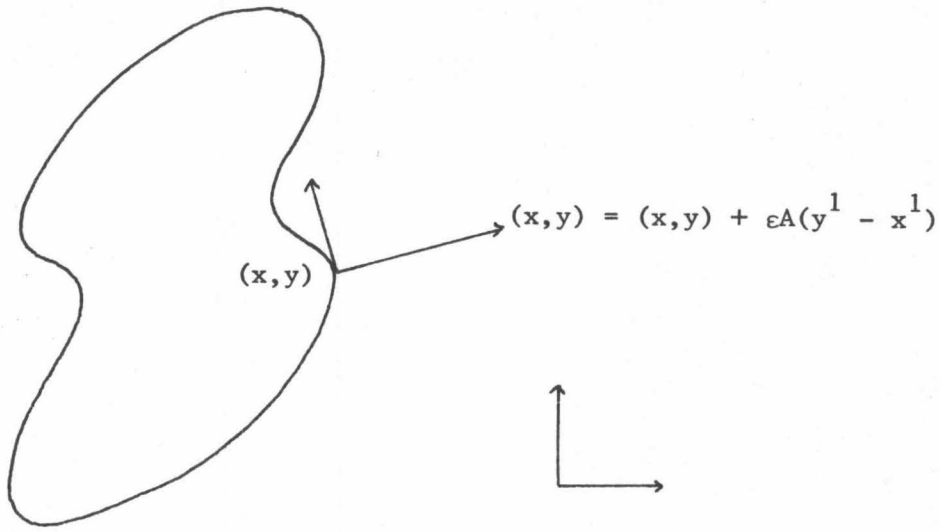


FIGURE 5.1

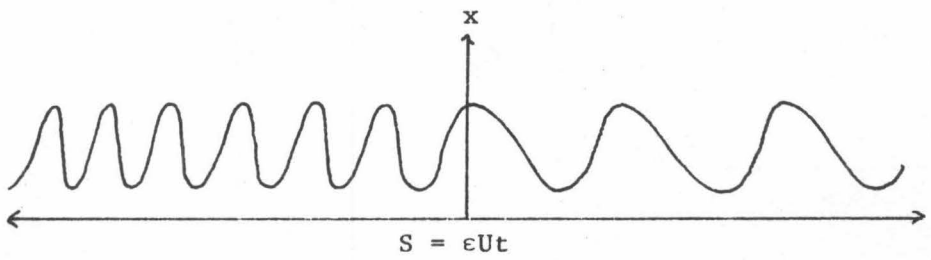


FIGURE 5.2

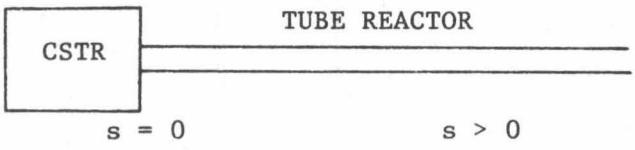


FIGURE 5.3

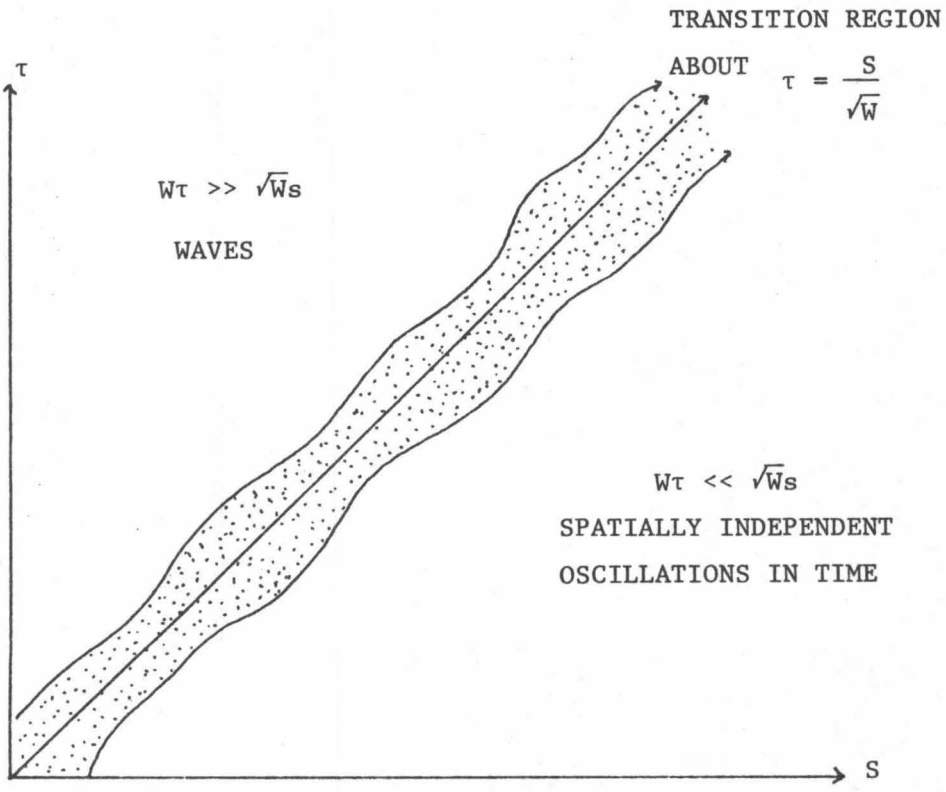


FIGURE 5.4

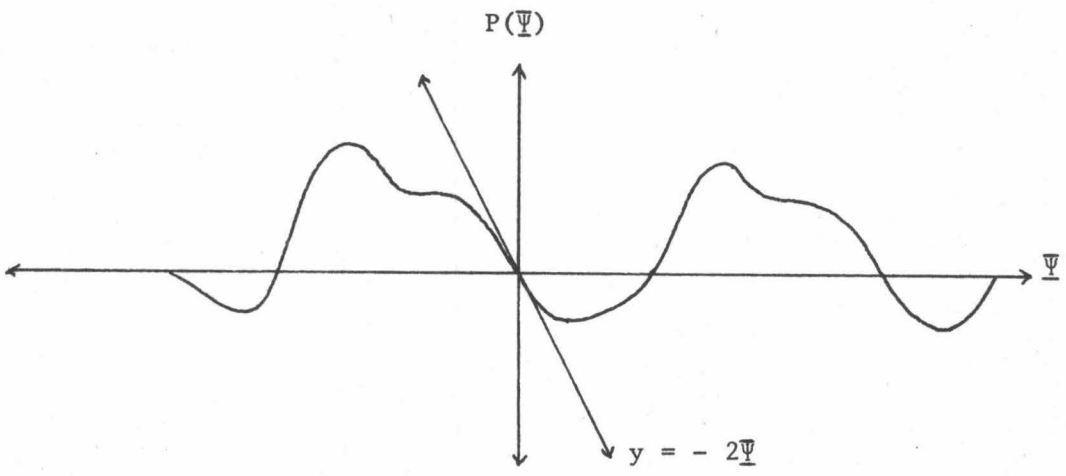


FIGURE 6.1

$$\frac{d\Psi}{d\tau} = k\{P(\Psi) - P\Psi_m)\} + \delta^2$$

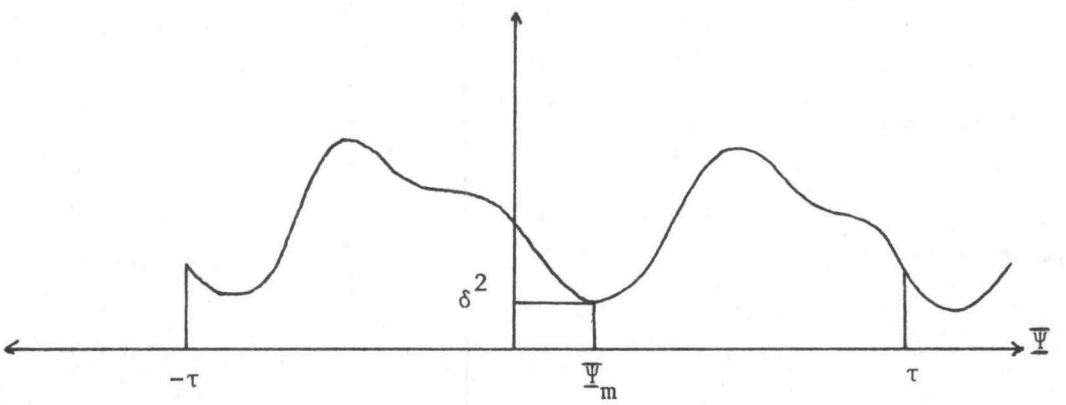


FIGURE 6.2

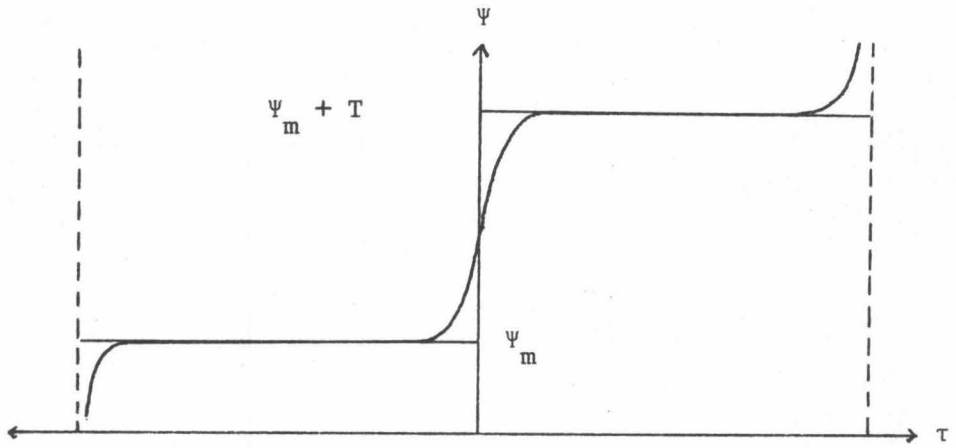


FIGURE 6.3

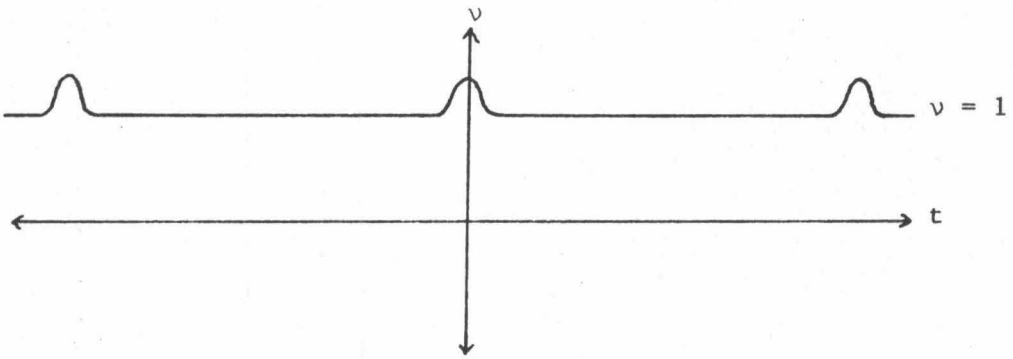


FIGURE 6.4

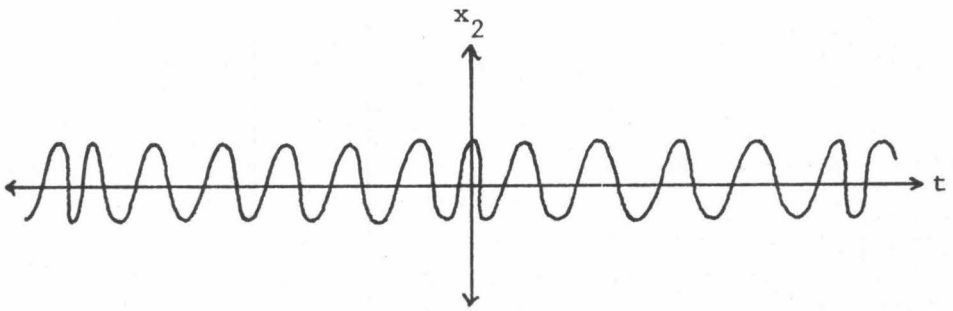


FIGURE 6.5

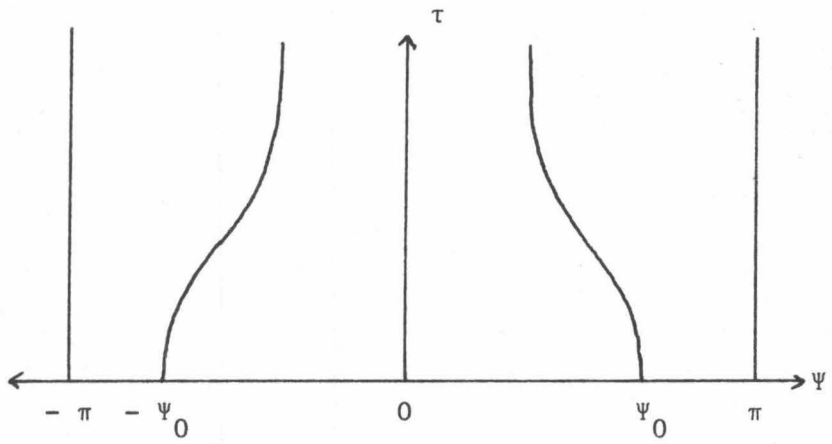


FIGURE 7.1

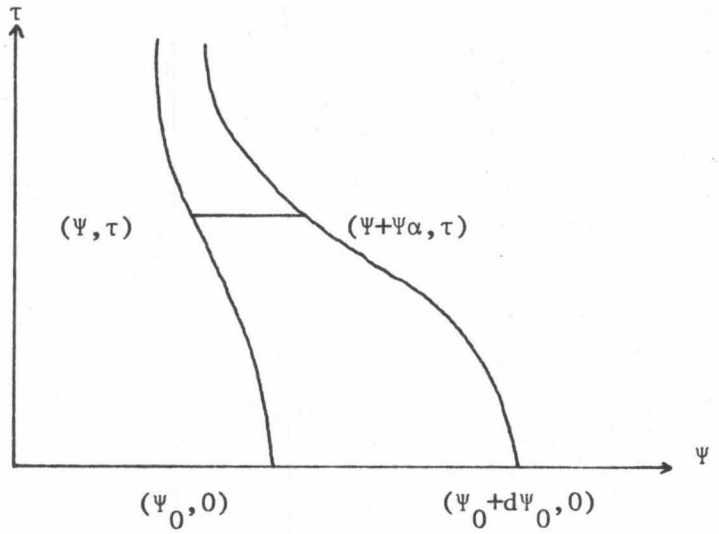


FIGURE 7.2

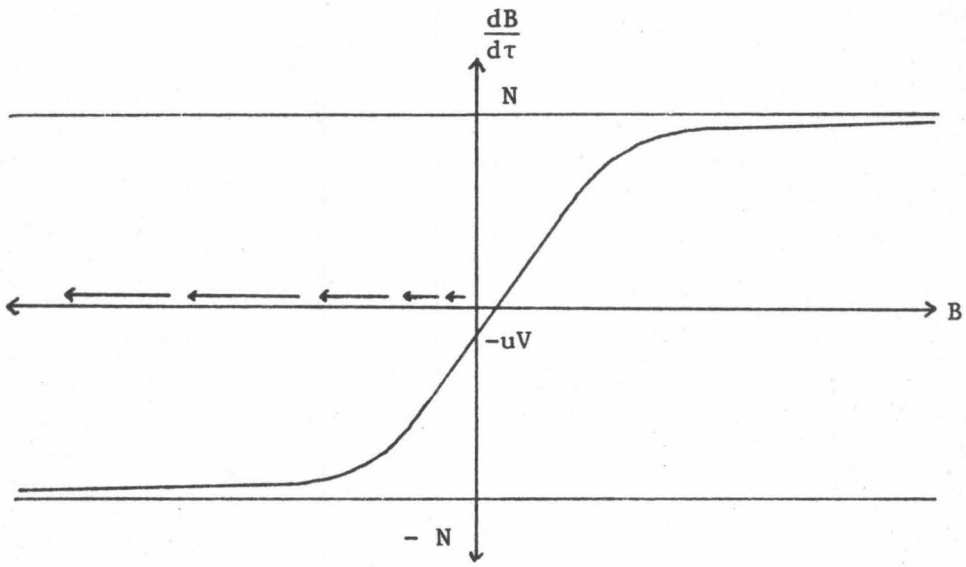


FIGURE 7.3

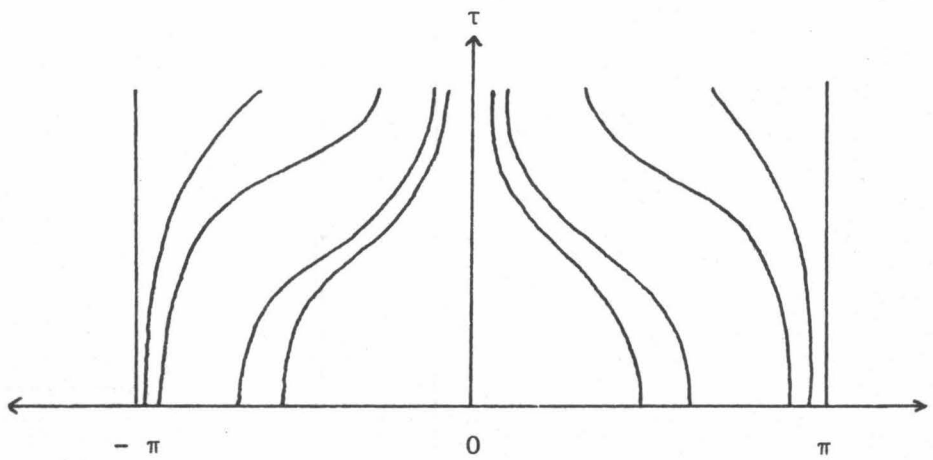
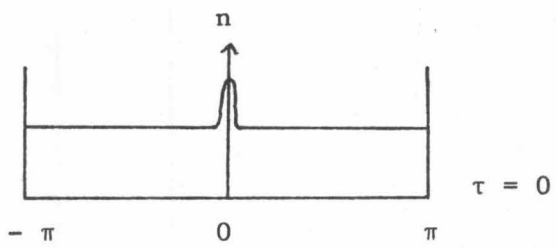


FIGURE 7.4



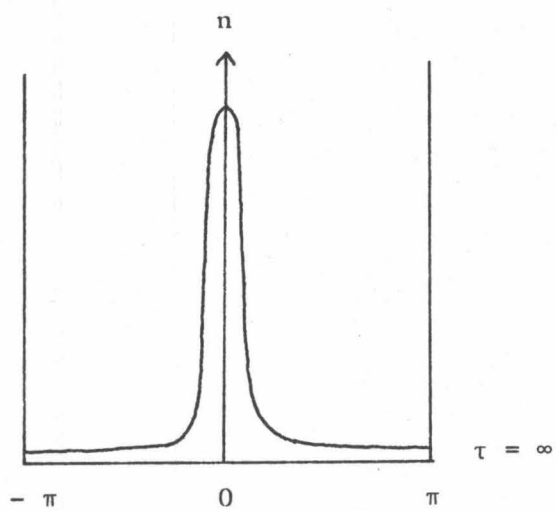


FIGURE 7.5

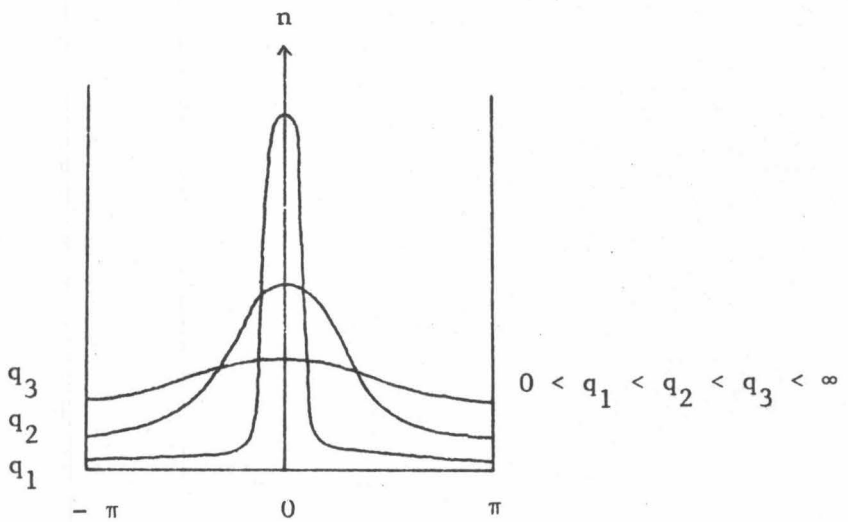


FIGURE 7.6

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