Cooperative phenomena in systems far from thermal equilibrium and in nonphysical systems

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This article consists of two parts. The first part presents a tutorial approach to cooperative phenomena in systems far from thermal equilibrium and in nonphysical systems. Particular emphasis is placed on the question of how order and self-organization may arise. The following example is treated among others: the ordered phase of the laser giving rise to both coherently oscillating atomic dipole moments and coherent light emission. A complete analogy of the laser light distribution function to that of the Ginzburg-Landau theory of superconductivity is found mathematically which allows us to interpret the laser threshold as a quasi-second-order phase transition with soft modes, critical slowing down, etc. Similar phenomena, again closely resembling phase transitions, are found in tunnel diodes and in the nonlinear wave interaction which occurs, for example, in nonlinear optics. Remarkable analogies between the instability of the laser and those in hydrodynamics are elaborated. While these phenomena show pronounced analogies to phase transitions in thermal equilibrium, there are further classes of instabilities and new phases which rather resemble hard excitations known in electrical engineering. Chemical oscillations are particularly important examples. In addition, the first part of this article contains the example of the cooperative behavior of neuron networks and shows the applicability of simple physical concepts, e.g., the Ising model, to the problem of the dynamics of social groups. All these above–mentioned examples demonstrate clearly that rather complex phenomena brought about by the cooperation of many subsystems can be understood and described by a few simple concepts. One of the main concepts is the order parameter; another is the adiabatic elimination of the variables of the subsystems, which is based upon a hierarchy of time constants present in most systems. The second part of this article gives a systematic account of the mathematical tools which allow us to deal with fluctuations. It contains the master equation, the Fokker–Planck equation, the generalized Fokker-Planck equation, and the Langevin equations, and gives several general methods for deriving the stationary and, in certain cases, the nonstationary solutions of master equations and the Fokker-Planck equations. Such general classes comprise those in which detailed balance is present or in which the coupling to the reservoirs is weak. In the quantum mechanical domain, the density matrix and the projection formalism for its reduction are presented. Finally, it is shown how the principle of quantum-classical correspondence allows us to translate quantum statistical problems completely into the classical domain.

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PART I: A TUTORIAL APPROACH

I. INTRODUCTION

We often analyze the properties of a system by decomposing it into its subsystems. In many cases we discover that these properties cannot be explained as mere random superimpositions of the effects of the sybsystems. Quite to the contrary, the subsystems seem to cooperate with each other in a well regulated manner. Furthermore, the behavior of the total system may show characteristic changes which can be described as a transition from disorder to order, or, as a transition from one state of order to a different one.

In physics there are numerous examples of such behavior, e.g. the ferromagnet, where the parallel alignment of the spins causes a macroscopic magnetization, or the superconductor which behaves as a quantum system with a macroscopic wavefunction. While these systems go into the ordered state when temperature is lowered, pronounced cooperative phenomena may also occur in physical systems far from thermal equilibrium, and may occur even in nonphysical systems. In physical systems far from equilibrium the ordered states are created and maintained by an energy flux passing through the system. Thus it is not surprising that such systems comprise active devices like lasers, tunnel diodes, Gunn oscillators, etc., which have technical applications.

It came as a surprise to many physicists, however, that there are profound analogies between the behavior of such systems and the behavior of conventional systems in thermal equilibrium. These analogies include phenomena characteristic of phase transitions, such as: symmetry breaking instabilities, critical slowing down, soft modes, critical fluctuations, etc. (for an explanation of these concepts see Sec. II). The discovery of these analogies have a number of independent sources and elaborations. These include Landauer's work (1961, 1962, 1967, 1971a, 1971b) on tunnel diodes and data processing, the work by Haken (1964, 1970), Martin (1965), Graham and Haken (1968, 1970), DeGiorgio and Scully (1970) and others dealing with lasers and related devices, and the work of Pytte and Thomas (1968, 1969) with respect to the Gunn effect, to mention a few examples.

The purpose of the present article is twofold.

(1) We want to show by means of examples selected from different disciplines how subsystems act to create order on a macroscopic scale.

(2) We want to develop the concepts which underlie all these seemingly quite different systems, including some biological and sociological models.

The systems with which we are concerned possess an enormous number of subsystems (or degrees of freedom). The determination of the detailed behavior of any individual subsystem is, in general, hopeless—but fortunately, this is not needed. We are interested in features only on a macroscopic scale. Thus, it is our task to select the *relevant* parameters and to do away with all unnecessary information. To achieve this goal, the concept of the *order parameter*, well-known in phase-transition theory, has turned out to be a very useful tool. For example, consider the mean field theory of the ferromagnet. In this theory direct interaction (caused by the Coulomb exchange interaction) between the spins is replaced by a two-step procedure: first a macroscopic quantity (the magnetization) is constructed, generated by the different spins; then this magnetization acts on each individual spin to tell each how to behave. The magnetization acts as an order parameter in two respects. It gives orders to the subsystems and it also describes the degree of order (it is zero in the disordered state and acquires a maximum value in the ordered state). The order parameter (or a set of such parameters) represents the behavior of the system on a macroscopic scale, and is thus a macroscopic variable.

Often the equations for such order parameters acquire a rather simple structure with respect to their time dependence. The reason for this is that the relaxation time of order parameters is usually much greater than those of the subsystems. Thus the subsystems can follow the "orders" of the order parameter adiabatically and the variables of the subsystem can be eliminated without increasing the degree of the time derivatives. The long relaxation time or, in other words, the long lifetime of the order parameter allows it to "slave" the subsystems (a technical expression from control systems engineering).

This concept of the order parameter also sheds new light on the problem of self-organization: the subsystems themselves create fictitious or real quantities which via feedback loops organize the behavior of the subsystems. It is nearly superfluous to say that there are close analogies between the equations of the order parameters we will obtain, and those of control circuits, e.g., in electrical engineering.

In certain classes of systems the disorder–order transitions are characterized by an infinite relaxation time at the transition without oscillations of the corresponding order parameter. In this case the above–mentioned analogy with phase transitions applies. An important difference should be mentioned, however. In usual phase-transition theory the use of the order parameter concept may break down close to the critical point, and has to be replaced by other methods, e.g., the scaling laws [see Kadanoff *et al.* (1967)] or Wilson's techniques (Wilson 1971a,b), yet this concept remains extremely useful for the systems treated in our article. One reason is that a thermodynamic limit in many cases is not required. Instead, a limit may even obscure a problem, e.g., the reliability of a device due to its finiteness. Furthermore, some of the phenomena depend on the geometry of the system. Let us discuss the phase-transition analogy to systems that are in and far from thermal equilibrium a bit further. Landauer suggested that a link among such systems is provided by the principle of detailed balance, and this conjecture has since been proven by Graham and Haken (1971a,b). It should be stated clearly, however, that this principle applies to systems in thermal equilibrium although it need not necessarily hold for other systems which may show more complexity. The situation is rather this: when a system far from thermal equilibrium becomes unstable with a soft mode, its dynamics is governed by a single degree of freedom and can often be described by a continuous Markov process. In such a case we may invoke the principle of detailed balance. Thus, close to such a point this principle holds to an excellent approximation, and it appears as a prerequisite for phase-transition-like behavior. In this case we now have a complete description, including the behavior in the transition region.

In general, however, the principle of detailed balance cannot be invoked for systems far from thermal equilibrium. This may easily be seen in the example of a three-level atom which is pumped to its uppermost level and which then undergoes further transitions between its levels. Further examples of the violation of this principle are provided by chemical oscillations. Here the situation is much less well understood and requires further developments. We hope that the degree of understanding of the various categories is clearly mirrored by our examples.

An adequate treatment of all these phenomena requires a statistical description which we have adopted throughout this article. We will see that the behavior of the systems is determined by some causal forces and fluctuating forces. The fluctuating forces which act on the order parameters are the trace left by the "underworld" of the subsystems (and other "reservoirs"). Our models will allow us to study in detail the interplay between the stochastic forces and the coherent forces, or, in a more philosophical language, the interplay between chance and necessity. The detailed mathematical apparatus for the models is developed in the second part of this article and includes results obtained very recently. This mathematical apparatus is also readily applicable to some biological problems, e.g., to the theory of evolution.

In conclusion, a word should be said of the relation of the approach presented in this article to approaches made within irreversible thermodynamics, or to still more advanced thermodynamical approaches like that by Glansdorff and Prigogine. In our approach we start from stochastic equations of motion either for microscopic systems or for systems described by order parameters. The thermodynamic approach begins with the assumption that there exists local thermodynamic equilibrium; this allows us to define quantities like entropy, so that the principle of excess entropy production (Glansdorff and Prigogine) can be applied. While this principle proves to be a useful tool in the "linear regime," its applicability to the "phase-transition" region which requires a truly nonlinear treatment seems to require further investigation.

II. SOME BASIC CONCEPTS[1]

A. The damped anharmonic oscillator

In this section we anticipate that the variables of the subsystems have already been eliminated and that we are dealing with the equations of the order parameter alone. A great many concepts can be exemplified by means of the damped anharmonic oscillator. As we will see later, its coordinate q may stand for the coordinate of a particle, for its velocity, for the size of the charge, for the magnetization, for the electric field strength or for many other quantities. We hope the following analysis will demonstrate how concepts from such different disciplines as nonlinear mechanics, electrical engineering, phase-transition theory, thermodynamics, fluid mechanics and other fields are linked together.

However, because this article is written primarily for physicists we first interpret q as the coordinate of a particle. We denote its mass by m, its damping constant by γ, the linear "restoring" force by $-\alpha q$, and we introduce the nonlinear restoring force $-\beta q^3$. The equation of motion reads

$$m\ddot{q} + \gamma\dot{q} = -\alpha q - \beta q^3. \tag{2.1}$$

The force

$$k(q) = -\alpha q - \beta q^3 \tag{2.2}$$

possesses a potential

$$k(q) = -(\partial V/\partial q), \tag{2.3}$$

where

$$V = \tfrac{1}{2}\alpha q^2 + \tfrac{1}{4}\beta q^4. \tag{2.4}$$

The potential is plotted as a function of the coordinate q for different values of α and β in Figs. 1 and 2. In the follow-

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[1] This paragraph is intended primarily for students. Experts may find it amusing to see how many concepts are brought out in this simple example.

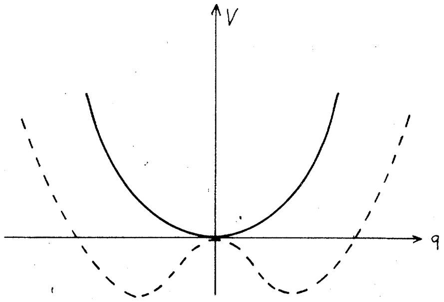

FIG. 1. The potential V (2.4) as a function of q for $\beta > 0$. Solid curve, $\alpha > 0$; dashed curve, $\alpha < 0$.

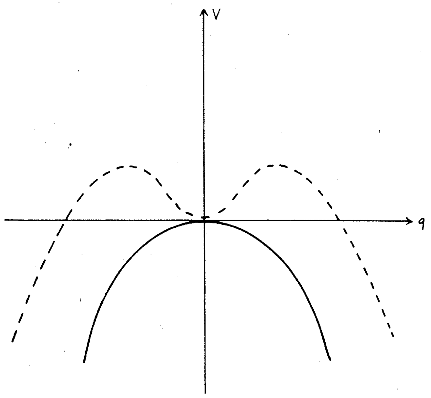

FIG. 2. The potential V (2.4) as a function of q for $\beta < 0$. Solid curve, $\alpha < 0$; dashed curve, $\alpha > 0$.

ing we will emphasize Fig. 1 where $\beta > 0$. Figures 1 and 2 allow us to discuss *global* and *local stability*.

(a) *Global stability*. In the case $\beta > 0$ the system is globally stable. Whereever the particle starts it comes to rest at a finite value of q. On the other hand we have global instability for $\beta < 0$.

(b) *Local stability*. Let us first consider the steady state characterized by

$$\dot{q} = \ddot{q} = 0. \tag{2.5}$$

Using Eq. (2.1) the states of stable or unstable equilibrium are then defined by

$$\alpha q + \beta q^3 = 0. \tag{2.6}$$

For $\alpha > 0$, we have the stable solution

$$q_0 = 0. \tag{2.7}$$

In the language of mathematicians, this state is an "attractor." For $\alpha < 0$ the state $q_0 = 0$ becomes unstable ("repeller"). Instead, we have now the two stable solutions

$$q_{1,2} = \pm(|\alpha/\beta|)^{1/2}. \tag{2.8}$$

With the transition from $\alpha > 0$ to $\alpha < 0$ the system passes through an instability by which the symmetry is broken. The particle is now either at q_1 or at q_2 [compare Eq. (2.8)]. (*Symmetry breaking instability*). Note, however, that on a global scale the potential is still completely symmetric. In fluid dynamics the change of one stability state to another is called an exchange of stabilities. The steady state, where $\alpha = 0$, $q = 0$, is a marginal state, i.e., it has neutral stability. In mathematics, the passing over from one stable state to two new ones is known as (Hopf) *bifurcation.*

As we will see later, fluctuations usually must be incorporated in the order parameter equations. Let us assume that the particle gets impulses of equal magnitude, but that it gets them randomly in forward or backward direction. These impulses are recognized by adding to Eq. (2.1) the random force

$$\phi(t) = \zeta \sum_j (-1)^{n_j} \delta(t - t_j), \tag{2.9}$$

where ζ stands for the size of the impulses, n_j is a random variable with values 0 or 1, and t_j is a random time sequence. δ is the usual Dirac function. We thus obtain

$$m\ddot{q} + \gamma\dot{q} = -\alpha q - \beta q^3 + \phi(t). \tag{2.10}$$

For the sake of simplicity we confine our following analysis largely to the heavily damped oscillator, in which case we can formally put $m = 0$. Introducing further the new quantities

$$\alpha/\gamma = a \qquad \beta/\gamma = b \qquad \phi/\gamma = F, \tag{2.11}$$

we may transform (2.10) into

$$\dot{q} = -aq - bq^3 + F(t). \tag{2.12}$$

We want to discuss this equation from various points of view. In Eq. (2.12) the explicit form of the fluctuating force (2.9) is not needed. What is needed are the correlation functions. Because impulses in the positive and negative direction are assumed of equal size we have

$$\langle F(t) \rangle = 0. \tag{2.13}$$

The brackets $\langle \cdots \rangle$ denote the statistical average over the direction of the impulses (i.e., n_j) and the times t_j. For more details about such averages consult Sec. X.A. In most applications the correlation function

$$\langle F(t) F(t') \rangle \tag{2.14}$$

is needed. Using the form

$$F(t) = F_0 \sum_j (-1)^{n_j} \delta(t - t_j), \tag{2.15}$$

one may show that

$$\begin{aligned} \langle F(t) F(t') \rangle &= F_0^2 \sum_j \overline{\delta(t - t_j)\delta(t' - t_j)} \\ &= (F_0^2/t_0)\delta(t - t') = C\delta(t - t'), \end{aligned} \tag{2.16}$$

where t_0 is the mean time between impulses.

Forces, whose second-order correlation function (2.16) is a δ function, are sometimes called Markovian in the literature. Some care should be exercised with this notation to avoid confusion with the concept of a "Markov process" (compare Chapter X). For a complete analysis of Eq. (2.12) we first put $F(t) = 0$. The time-dependent solution of $\dot{q} = -aq - bq^3$ reads

$$q(t) = \pm(a)^{1/2}\{\exp[2a(t-t')] - b\}^{-1/2} \quad \text{for} \quad a > 0 \tag{2.17}$$

and

$$q(t) = \pm(|a|)^{1/2}\{b - \exp[-2|a|(t-t')]\}^{-1/2} \quad \text{for} \quad a < 0. \tag{2.18}$$

Note that a has the meaning of an inverse relaxation time. In both cases $a \gtrless 0$, q tends to its equilibrium value. Because in more general cases of order-parameter equations an explicit solution cannot be found, we must discuss further tools for studying the motion of the particle. We first investigate *local stability* by the *method of linearization.*

We define the coordinate q_s of the steady state by $\dot{q}_s = 0$ and put

$$q = q_s + \delta q. \tag{2.19}$$

Let us first linearize Eq. (2.12) around $q_s = 0$ which yields

$$\delta\dot{q} = -a\delta q \tag{2.20}$$

with the solution

$$\delta q = A\exp(-\Gamma t), \qquad \Gamma = a. \tag{2.21}$$

For $a > 0$ the system is stable, for $a = 0$ we have a marginal state (neutral stability), for $a < 0$ the system becomes unstable. When a approaches 0, the relaxation constant Γ tends also to 0: we have the phenomenon of *critical slowing down* connected with a *soft mode.*[2] If on the other hand $a < 0$, the coordinate of the stable point is

$$|q|_s = (|a|/b)^{1/2}. \tag{2.22}$$

Inserting

$$q = q_s + \delta q \tag{2.23}$$

into $\dot{q} = -aq - bq^3$ yields

$$(d/dt)\delta q = -2|a|\delta q, \tag{2.24}$$

so that the relaxation time

$$\tau = (2|a|)^{-1}. \tag{2.25}$$

We consider the *fluctuations of q in the linearized theory* and solve the equation ($a \geq 0$)

$$(d/dt)\delta q + a\delta q = F(t), \tag{2.26}$$

which yields

$$\delta q = \exp(-at)\int_{t_0}^{t}\exp(a\tau)F(\tau)\,d\tau. \tag{2.27}$$

A measure for the temporal behavior of the system (the particle) is the correlation function of its coordinate. Inserting Eq. (2.27) into

$$\langle\delta q(t)\delta q(t')\rangle \tag{2.28}$$

yields after elementary calculations (for $t_0 \rightarrow -\infty$)

$$\langle\delta q(t)\delta q(t')\rangle = (C/2a)\exp[-a(t-t')]; \qquad t \geq t'. \tag{2.29}$$

From Eq. (2.28) it is evident that as $a \rightarrow 0$ not only the relaxation time $\tau = (1/\Gamma)$ becomes infinite, but also the coordinate fluctuation ("*critical fluctuations*"). It is, however, an important point that the divergence of Eq. (2.28) for $a \rightarrow 0$ is caused by the linearization procedure, or, in other words: while the fluctuations δq for $a > 0$ or $a < 0$ are finite and can in many cases be neglected, the linearization procedure breaks down near the point $a = 0$. In the exact theory, which avoids linearization, it remains true, however, that at the critical point $a = 0$ the fluctuations in δq become large. In such a region the correlation function $(t > t')$

$$\langle q(t)q(t')\rangle \tag{2.30}$$

can be found only by computer solution, even in our simple example. The concepts of critical slowing down, soft mode, critical fluctuations, and symmetry breaking, belong to the standard repertoir of phase-transition theory.

We now proceed to *some methods of statistical mechanics.* Equation (2.12) may be considered as an extension of the *Langevin equation of Brownian motion*

$$\dot{q} = -aq + F(t). \tag{2.31}$$

Note that q is now interpreted as the velocity of a particle. While it is quite simple to solve

$$\dot{q} = -aq - bq^3 + F(t) \tag{2.32}$$

in the linearized domain, its solution becomes a formidable task even for this very simple case if the nonlinearity is kept. It is advantageous to proceed to the *Fokker–Planck equation* which is given by

$$\dot{f}(q,t) = -(\partial/\partial q)(K(q)f) + \tfrac{1}{2}(\partial^2/\partial q^2)(Q(q)f). \tag{2.33}$$

Here $f(q,t)\,dq$ is the probability of finding the particle with coordinate q in the interval $q\cdots q + dq$ at a time t. The

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[2] If at the instability undamped *oscillations* occurs, we are dealing with a *hard excitation.*

general formulation of a Fokker–Planck equation will be given in Sec. X. Here we only give a recipe which allows us to determine $K(q)$, $Q(q)$. The so-called drift coefficient K is defined by

$$K(q) = \lim_{t\to 0}(1/t)\langle(q(t) - q(0))\rangle; \tag{2.34}$$

the diffusion coefficient by

$$Q(q) = \lim_{t\to 0}(1/t)\langle(q(t) - q(0))^2\rangle. \tag{2.35}$$

In both cases one has to imagine that Eq. (2.32) is solved for a time interval which still comprises many pushes of $F(t)$ but is small compared to the overall motion of the system. In the present case one readily finds that $K(q)$ is identical with the force $k(q)$ introduced in Eq. (2.2):

$$K(q) = -aq - bq^3 = -(\partial V/\partial q), \tag{2.36}$$

and that

$$Q(q) = C, \tag{2.37}$$

where C is defined as the coefficient in the correlation function (2.16). The Fokker–Planck equation (2.33) thus reads

$$\dot{f}(q,t) = -\frac{\partial}{\partial q}\left\{\left(-\frac{\partial V}{\partial q}\cdot f\right) - \tfrac{1}{2}C\frac{\partial f}{\partial q}\right\}. \tag{2.38}$$

Having in mind that f has the meaning of a (probability) density, Eq. (2.38) has the form of a conservation law: Denoting the probability current by j, we obtain

$$\dot{f} = -(\partial/\partial q)\, j. \tag{2.39}$$

In the stationary state

$$\dot{f} = 0 \tag{2.40}$$

we readily find the solution

$$\begin{aligned} j = 0, \quad f &= \mathfrak{N}\exp\left(-\frac{2V}{C}\right) \\ &= \mathfrak{N}\exp\{-(2/C)(\tfrac{1}{2}aq^2 + \tfrac{1}{4}bq^4)\}, \end{aligned} \tag{2.41}$$

where we have taken into account that f vanishes at infinity, because f must be normalizable.

The distribution function f is of great importance because it governs the *stability*, the *fluctuations* and the *dynamics* of the system.

(a) *The stability.* A comparison with our previous considerations reveals that those systems are globally stable in which f is normalizable. We call a point q_0 locally stable if the exponent in Eq. (2.41) has a local maximum at that point. (This maximum can be also metastable if there are other maxima which yield a higher probability f). V serves as a *Liapunov function* V_L which fulfills the following criteria: [put $V_L(q) = V(q) - V(q_0)$!].

(1) $V_L(q)$ and its first derivative are continuous in a region surrounding q_0,

(2) $V_L(q_0) = 0$,

(3) in a region surrounding q_0, $V_L(q) > 0$,

(4) $\dot{V}_L = k\,\mathrm{grad} V_L \leqq 0$, (2.42)

where

$$\dot{q} = k(q). \tag{2.43}$$

Then the stability criterion of Liapunov states: If there exists in a region surrounding q_0 a Liapunov function $V_L(q)$, then q_0 is stable.

(b) *The fluctuations.* Expanding the exponent $V(q)$ in F (2.41) about the stable state of the system using

$$q = q_s + \delta q$$

yields an expression for the probability of finding a fluctuation of size δq.

$$\begin{aligned} &f(q) \\ &= \mathfrak{N}\exp - 2\left\{\frac{1}{C}V(q_s) + \frac{1}{2C}\left.\frac{\partial^2 V(q)}{\partial q^2}\right|_{q_s}(\delta q)^2\right\}. \end{aligned} \tag{2.44}$$

(c) *the dynamics.* Here $V(q)$ (or V/C) can serve as a criterion for the development of the system. Evidently the system with initial state q_a develops in time such that at a later time

$$V(q) < V(q_a) \tag{2.45}$$

holds. Furthermore, from the knowledge of $V(q)$ one may deduce the equation of motion without fluctuating forces by means of

$$\dot{q} = -(\partial V/\partial q).$$

We now abandon the description of our problem in the terminology of mechanics and statistical mechanics and turn to *thermodynamics*, where we consider the problem of Brownian motion. We assume that the random pushes exerted by the random force $F(t)$ on the particle are caused by a "heatbath" in thermal equilibrium into which our particle is immersed. To obtain the correct physical properties of the fluctuating force we must go back to Eq. (2.10) where we put $\alpha = \beta = 0$, assuming that a coherent force $k(q)$ does not influence the random impulses supplied by the heatbath. The resulting equation has the form (2.26) provided we make the following replacements in (2.26)

$$q \to \dot{q}, \qquad a \to (\gamma/m), \qquad F \to (\phi/m).$$

Using (2.27), (2.28), (2.29) and putting

$$\langle\phi(t)\phi(t')\rangle = C'\delta(t - t'), \tag{2.46}$$

we obtain (with $v \equiv q$)

$$(m/2)\langle v^2\rangle = (C'/4\gamma). \tag{2.47}$$

On the other hand, we know that in thermal equilibrium

$$(m/2)\langle v^2\rangle = \tfrac{1}{2}k_BT, \tag{2.48}$$

where k_B is the Boltzmann constant, and T the absolute temperature. Comparing Eq. (2.48) with (2.47) leads to the very important relation

$$C' = 2\gamma k_BT. \tag{2.49}$$

This states that the correlation constant C' of the fluctuating forces and the damping constant γ are connected with each other by necessity. Passing from the fluctuating force ϕ to F according to Eq. (2.11), and using Eq. (2.49), we obtain the constant C occuring in Eq. (2.16) as

$$C = C'/\gamma^2 = 2k_BT/\gamma. \tag{2.50}$$

Such *relations between fluctuation and dissipation* are of fundamental importance for all systems we will consider, be they quantum systems or classical systems, or systems in or away from thermal equilibrium. Relations which generalize Eq. (2.50) to such systems have been found more recently (see Sec. XII).

In later applications we will see that establishing functions of the form (2.41) or its generalization is one of the main goals of the theory. In thermodynamics we may determine the probability distribution function f directly by general principles rather than by solving the Fokker–Planck equation.

To this end we remind the reader of the relation between *entropy and probability.* Consider quite generally a subsystem within a closed system. The state of the subsystem is described by the parameter q which together with its temperature determines its energy. We permit thermal energy to be exchanged with the rest of the total system as the subsystem is subject to coherent forces. According to thermodynamics, the probability of finding the subsystems in the interval from q to $q + dq$ is given by

$$f(q)\,dq = \mathfrak{N} \exp(k_B^{-1}S(q))\,dq, \tag{2.51}$$

where $S(q)$ is the entropy, k_B is again the Boltzmann constant, and $\mathfrak{N}$ is the normalization factor defined by

$$\mathfrak{N} = \int \exp(k_B^{-1}S(q))\,dq. \tag{2.52}$$

We show in a well-known manner how to determine $S(q)$ directly in the present case where q is identified with the previous coordinate q. We compare the two states $q = 0$ and $q \neq 0$ having the same energy. The energy needed to bring the particle from $q = 0$ to q (neglecting kinetic energy) is

$$V(q) = \tfrac{1}{2}\alpha q^2 + \tfrac{1}{4}\beta q^4. \tag{2.53}$$

Because the final state is supposed to have the same energy as the initial state we must take the energy (2.53) away from the system in the form of heat, i.e.,

$$S(q) = \int \frac{dQ_{rev}}{T} = -\frac{V(q)}{T}. \tag{2.54}$$

Application of Eq. (2.51) to our present case yields

$$f(q)\,dq = \mathfrak{N} \exp(-(1/k_BT)V(q))\,dq. \tag{2.55}$$

This result is identical with Eq. (2.41), provided we use Eq. (2.11) and the relation (2.50) between dissipation and fluctuation coefficients. Let us now expand $V(q)$ around its equilibrium point q_0 in powers of δq. This yields apparently the *probability $w(q)$ for a fluctuation of size δq.* This *Einstein relation* yields

$$w(q) \sim \exp\left(\frac{1}{2k_B}\frac{\partial^2 S}{\partial q^2}(\delta q)^2\right). \tag{2.56}$$

(Note that the derivative of V vanishes at the equilibrium point.)

Our example of the overdamped anharmonic oscillator is also a simple example for the demonstration of the *Landau theory of phase transitions.* It starts with the expression[3]

$$f(q) = N\exp(S/k_B), \tag{2.57}$$

and tries to determine S as a function of the "order parameter" q by symmetry arguments. Particular attention is paid to the case in which an instability for $a = 0$ occurs. The potential V possesses mirror symmetry with respect to the V axis, i.e., it remains invariant under the transformation $q \rightarrow -q$. Because the probability distribution must have the same invariance as the problem, S must be also an even function of q which can be expanded around the equilibrium value $q = 0$ as

$$S = d_1q^2 + d_2q^4 + \cdots. \tag{2.58}$$

Apparently the first two members of S already yield the correct potential (2.53), though in general the explicit form of the coefficients d_1, d_2 remains unknown in the Landau theory. In cases similar to our present problem, one may deduce, at least qualitatively, the dependence of d_1, d_2 on some of the important constants of the problem, in particular on the constant a. If a changes its sign the total symmetry remains but a new state occurs with new equilibrium positions. We therefore expect $d_1 \propto a$ in agreement with our previous results.

B. Some general conclusions

So far we have discussed a very simple system in thermal equilibrium. In the next paragraphs we will demonstrate by explicit examples that we are led to equations of the form

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[3] Depending on the physical situation, S must be replaced, e.g, by the free energy or some other thermodynamic potential.

(2.12) or its generalization to many coordinates for systems which are far from thermal equilibrium. In these cases q may represent quite different quantities, e.g., the laser light field, electric currents, velocity fields in fluids, concentrations of chemical reactants, etc. The stable states $q = q_s \neq 0$ are now maintained by a balance between energy input and dissipation. Most important for our subsequent treatment will be the fact that a great deal of the above analysis applies equally well to these more general cases. We briefly give a review of what has been achieved and which problems are still unsolved. The full mathematical apparatus will be developed in Part II of this review article.

(1) *Equations of motion.* Let the system be described by the order parameters $q_1, \cdots, q_n$ (which may also depend on a continuous index n).
In many cases, Langevin equations of the type

$$\dot{q}_j = k_j(q_1, \cdots, q_n) + F_j(t) \tag{2.59}$$

can be derived. These equations may be generalized to the quantum case, where q and F become operators. Both for classical and quantum systems there exist general relations between fluctuation and dissipation. Local stability may be studied by the method of linearization or by the Liapunov theory. A classification of critical points (if k_j can be derived from a potential) has been achieved by Thom (1972). However, we will not consider his work in this article. From Eq. (2.59) one may deduce a Fokker–Planck equation (or a generalized Fokker–Planck equation). Such an equation can also be derived from the density matrix equation through the principle of quantum-classical correspondence.

(2) *Methods of solution.* As we have seen, a great number of conclusions, particularly concerning critical points (in our example $a = 0$), can be drawn if the stationary solution of the Fokker–Planck equation is known. Explicit stationary solutions of the Fokker–Planck equation are known in the following cases:

(a) if the drift coefficients (compare (2.33), (2.34)) are linear in the coordinates and if the diffusion coefficients are independent of the coordinates,
(b) if the system shows detailed balance,
(c) if the system is weakly coupled to reservoirs,
(d) if the system is far from critical points showing just "normal fluctuations" (more precisely: *normally distributed* fluctuations). Time-dependent solutions may be found quite generally for (a) and (d), and, to some extent, for (c). In general, however, evaluation of time-dependent correlation functions requires numerical methods or certain approximation schemes.

The examples which follow will show that the analysis of our simple example above (including concepts like critical slowing down and stability) apply in many cases to systems far from thermal equilibrium as described by a variety of order parameters. There remain, on the other hand, other classes which at the present time are less understood, at least so far as fluctuations are concerned. These classes are characterized by hard excitations (in the terminology of electrical engineers) and by "cyclic balance," a concept introduced by Tomita (1973).

III. COOPERATIVE EFFECTS IN THE LASER

The laser is today one of the best understood many-body problems.[4] It is a system far from thermal equilibrium and it allows the study of cooperative effects in great detail. The essential feature to be understood about the laser is the following: If the laser atoms are pumped only weakly by external sources, the laser acts as an ordinary lamp. The atoms emit waves with random phases independently of each other. The coherence time of about 10^{-11} sec. is evidently on a microscopic scale. The atoms, visualized as oscillating dipoles, are oscillating completely at random. If the pump strength is increased, within a very sharp transition region the linewidth of the laser light may suddenly become of the order of one cycle per second. The phase of the field then remains unchanged on a macroscopic scale of 1 sec. Thus the laser is evidently in a new highly ordered state on a macroscopic scale. The atomic dipoles now all oscillate in phase, though they are excited by the pump completely at random. The extraordinary coherence of laser light is brought about by the cooperation of the atomic dipoles.

Let us now consider the laser in more detail. We take as an example the solid state laser which consists of a set of laser-active atoms embedded in a solid state matrix. As usual we assume that the laser end faces act as mirrors serving two purposes: they select modes in the axial direction and with discrete cavity frequencies. In our model we will treat atoms with two energy levels. In thermal equilibrium the levels are occupied according to the Boltzmann distribution function. The excited atoms form an inverted population which can be described by a negative temperature. The atoms now start to emit light which is eventually absorbed by the surroundings, whose temperature is much smaller than $\hbar\omega/k_B$ (where ω is the light frequency of the atomic transition and k_B is Boltzmann's constant), so that we may put this temperature ≈ 0. From a thermodynamic point of view the laser is a system (composed of the atoms and the field) which is coupled to reservoirs at different temperatures. Thus the laser is a system far from thermal equilibrium. Nevertheless we want to demonstrate that it shows all the features of a second-order phase transition.[5]

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[4] For a detailed account of the various aspects of laser theory, see Haken (1970) and Sargent, Scully, and Lamb (1974). These works include in particular the quantum statistics of the single mode laser, which is also treated by Lax (1968), Lax and Zwanziger (1973), and Louisell (1973). We do not intend to duplicate these works here, but rather to present those aspects of laser theory which are the most relevant ones in the present context. Our analysis is mainly based on our previous papers (Haken, 1962, 1964, 1965, 1966, 1969, 1970a, b, c; Arzt *et al.*, 1966, Graham and Haken, 1968, 1970), with particular emphasis on an interpretation in the spirit of the present article. From a mathematical point of view, our approach (as well as essential parts of Lax's and Louisell's work) is mainly based on the Langevin and Fokker–Planck equations referring to field amplitudes, while that of the Scully–Lamb theory uses the master equation which is dealt with in the photon number presentation. For further references consult the text and, in particular, the above mentioned books and articles.

[5] We do not enter into the discussion on the existence of the thermodynamic limit. Suffice it to say here that the single mode laser with the number of atoms N tending to infinity possesses such a limit, causing a sharp transition at the laser threshold (Dohm, 1972a, b).

A. Equations of classical dispersion theory

The mathematical description we will employ is somewhat reminiscent of the classical dispersion theory, which may be characterized as follows: The electric field strength obeys the wave equation

$$-\Delta\mathbf{E}+\frac{1}{c^2}+\ddot{\mathbf{E}}\frac{4\pi\sigma_c}{c^2}\dot{\mathbf{E}}=-\frac{4\pi}{c^2}\ddot{\mathbf{P}}, \tag{3.1}$$

where σ_c is the conductivity which describes the damping of the field, and P is the macroscopic polarization. Thinking of atoms dispersed in a medium, we may represent the polarization as a sum over the individual atomic contributions at sites $\mathbf{x}_\mu$ by

$$\mathbf{P}(\mathbf{x},t)=\sum_\mu\delta(\mathbf{x}-\mathbf{x}_\mu)\,\mathbf{r}_\mu(t), \tag{3.2}$$

where $\mathbf{p}_\mu$ is the dipole moment of atom μ. The field equation (3.1) is supplemented by the equation of the atom, μ,

$$\ddot{\mathbf{p}}_\mu+2\gamma\dot{\mathbf{p}}_\mu+\nu^2\mathbf{p}_\mu=(e^2/m)\mathbf{E}(\mathbf{x}_\mu,t), \tag{3.3}$$

where γ is the damping constant of the atoms.

B. The laser equations

While in a fully quantum mechanical treatment Eq. (3.1) may essentially be kept, Eq. (3.3) must be replaced by the quantum mechanical treatment of the single atom. Because the procedure has been described elsewhere and would take us far too much space, we present here only the relevant features. The electric field strength may be expanded into cavity modes in the form

$$\mathbf{E}(\mathbf{x},t)$$
$$=i\sum_\lambda\{(2\pi\hbar\omega_\lambda/V)^{1/2}\exp(i\mathbf{k}_\lambda\mathbf{x})b_\lambda-\text{c.c.}\}, \tag{3.4}$$

where for simplicity we assume running waves. Here λ is an index distinguishing the different modes, ω_λ is the mode frequency, V the volume of the cavity, $\mathbf{k}_\lambda$ the wave vector, b_λ and b_λ^+, in the classical description, are time-dependent amplitudes and, in the quantum mechanical description, are the creation and annihilation operators of photons. Though the analysis goes through in a completely quantum mechanical fashion it is perhaps more instructive to use a classical interpretation.[6] Anticipating that the dipole moments oscillate around a mean frequency ν, we use the decomposition

$$p_\mu=p_\mu^++p_\mu^-, \tag{3.5}$$

with

$$p_\mu^\pm\propto\exp(\mp i\nu t). \tag{3.6}$$

We now proceed to dimensionless quantities α_μ, α_μ^+ by putting

$$\mathbf{p}_\mu^{(+)}=\boldsymbol{\Theta}_{21}\alpha_\mu,\qquad\mathbf{p}_\mu^{(-)}=\boldsymbol{\Theta}_{21}^*\alpha_\mu^+, \tag{3.7}$$

where $\boldsymbol{\Theta}_{21}$ is the dipole moment matrix element between the two atomic levels. For the experts we mention that α_μ^+, α_μ may be interpreted as rising and lowering operators of the atom μ. (Their explicit definition is as follows: We use second quantization and denote the creation operator of an electron in the level j of the atom μ by $a_{j\mu}^+$, the corresponding annihilation operator by $a_{j\mu}$. Then $\alpha_\mu^+=a_{2\mu}^+a_{1\mu}$ and $\alpha_\mu=a_{1\mu}^+a_{2\mu}$.) We further denote the population of the levels 2 and 1 of atom μ by $N_{2,\mu}$ and $N_{1,\mu}$ respectively, and put $\sigma_\mu=(N_{2,\mu}-N_{1,\mu})$ or using $a_{j\mu}^+$, $a_{j\mu}$: $\sigma_\mu=a_{2\mu}^+a_{2\mu}-a_{1\mu}^+a_{1\mu}$. Denoting the coupling constants between field mode λ and atom μ by $g_{\mu\lambda}$, the Hamiltonian of the "proper laser system," field and atoms, becomes

$$H=\sum_\lambda\hbar\omega_\lambda b_\lambda^+b_\lambda+\tfrac{1}{2}\hbar\nu\sum_\mu\sigma_\mu+\hbar\sum_{\mu\lambda}(g_{\mu\lambda}^*b_\lambda\alpha_\mu^++\text{h.c.}). \tag{3.8}$$

From the Hamiltonian we may proceed to Heisenberg equations of motions for b_λ, b_λ^+, α_μ^+, α_μ, σ_μ. The structure of these equations is roughly analogous to those of Eqs. (3.1) and (3.3), if use of the relations (3.2), (3.4)–(3.7) is made. We hasten to remark that the proper laser system is still coupled to individual reservoirs: in the case of the field, for example, to currents in the mirrors, while in the case of the atomic field, to lattice vibrations or nonlasing field modes. Thus the Hamiltonian of the total system comprises not only Eq. (3.8), but also the interaction Hamiltonian of these reservoirs. By methods which we will describe in detail in Sec. 12, the reservoir coordinates may then be eliminated, leaving their trace in the equations of motion by causing damping and fluctuations.

We will not dwell, however, on these details but rather on the basic equations of motion. We have equations for the field amplitudes b_λ^+, for the dipole moments α_μ^+, and the inversion σ_μ.

1. Field equations

The equation for the field amplitude is:

$$\dot{b}_\lambda^+=(i\omega_\lambda-\kappa_\lambda)b_\lambda^++i\sum_\mu g_{\mu\lambda}^*\alpha_\mu^++F_\lambda^+(t). \tag{3.9}$$

Here ω_λ is the mode frequency, κ_λ is the decay constant of mode λ if left alone in the cavity without laser action, while F_λ^+ is a stochastic force which occurs necessarily, due to the unavoidable fluctuations when dissipation is present. In the present case these fluctuating forces are a consequence of quantum mechanical consistency (compare the second part of this article).

2. Matter equations

a. Equation for the atomic dipole moments

The equation for the atomic dipole moment is:

$$\dot{\alpha}_\mu^+=(i\nu-\gamma)\alpha_\mu^+-i\sum_\lambda g_{\mu\lambda}b_\lambda^+\sigma_\mu+\Gamma_\mu^+(t). \tag{3.10}$$

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[6] The method of quantum classical correspondence even allows the replacement of quantum mechanical equations by classical equations, either exactly or with well defined approximations (see Sec. XVI).

Here ν is the central frequency of the atom, γ is its linewidth caused by the decay of the atomic dipole moment, while the $\Gamma_\mu{}^+(t)$'s are stochastic forces.

b. Equation for the atomic inversion

The equation for atomic inversion is:

$$\dot{\sigma}_\mu = \gamma_{11}(d_0 - \sigma_\mu) + 2i \sum_\lambda (g_{\mu\lambda}\alpha_\mu b_\lambda{}^+ - \text{c.c.}) + \Gamma_{\sigma,\mu}(t). \tag{3.11}$$

Here d_0 is an equilibrium inversion which is caused by the pumping process and incoherent decay processes if no laser action takes place, γ_{11} is the relaxation time after which the inversion comes to an equilibrium, and the $\Gamma_{\sigma,\mu}$'s are again fluctuating forces.

Let us first consider the character of the equations (3.9) to (3.11) from a mathematical viewpoint. They are coupled, first-order differential equations for many variables. Even if we confine ourselves to the modes within an atomic linewidth, this may contain dozens to thousands of modes. Furthermore, there are typically 10^{14} laser atoms or many more, so that the number of variables of the system (3.9) to (3.11) is enormous. Also the system is nonlinear because of the terms $b^+\sigma$ in (3.10), and αb^+, $\alpha^+ b$ in (3.11). We will see in a moment that these nonlinearities play a crucial role and must not be neglected. Last but not least, the equations contain stochastic forces. Thus, at a first sight, the solution of our problem seems rather hopeless.

C. The order parameter concept

A discussion of the physical content of the equations (3.9) to (3.11) will help us to cut down the problem, and to solve it completely. Equation (3.9) describes the temporal change of the mode amplitude under two forces: (1) a driving force stemming from the oscillating dipole moments ($\alpha_\mu{}^+$) quite in analogy to the classical theory of the Hertzian dipole [compare also Eq. (3.1)], and, (2) a stochastic force F^+. Equations (3.10)–(3.11) describe the reaction of the field on the atoms.

Let us first assume that in (3.10) the inversion σ_μ is kept constant. Then b^+ acts as a driving force on the dipole moment in analogy to the classical equation (3.3) where E acts as a driving force on p_μ. If the driving force has the correct phase and is near resonance, we expect a feedback between the field and the atoms, or, in other words, we obtain stimulated emission. This stimulation process has two opponents. On the one hand, the damping constants κ and γ will tend to drive the field to zero; on the other hand the fluctuating forces will disturb the total emission process by their stochastic action. Thus we expect a damped oscillation.

As we will see more explicitly below, if we increase σ_μ, the system becomes unstable suddenly with exponential growth of the field and correspondingly of the dipole moments. Usually it is just a single field mode which first becomes undamped or, in other words, unstable. In this instability region the internal relaxation time is apparently very long. This makes us anticipate that the mode amplitudes, which become undamped, may serve as the order parameters. These slowly varying amplitudes now slave the atomic system. The atoms have to obey the orders of the order parameters as described by the right-hand sides of Eqs. (3.10) and (3.11). If the atoms follow without delay, the orders of the order parameter, we may eliminate the "atomic" variables α^+, α, σ, adiabatically, obtaining equations for the order parameters b_λ alone. These equations describe most explicitly the competition of the order parameters among each other, finally obeying the order parameter which wins the competition. In order to learn more about this mechanism we first anticipate that one $b_\lambda{}^+$ has won the competition and we confine our analysis to this single mode case.

D. The single mode case

We drop the index λ in Eqs. (3.9)–(3.11), assume exact resonance $\omega = \nu$, and eliminate the time dependence by the substitutions

$$b^+ = \tilde{b}^+ \exp(i\omega t), \qquad \alpha_\mu{}^+ = \tilde{\alpha}_\mu{}^+ \exp(i\nu t),$$
$$F^+ = \tilde{F}^+ \exp(i\omega t), \tag{3.12}$$

where we finally drop the tilde. The equations we consider are then

$$\dot{b}^+ = -\kappa b^+ + i \sum_\mu g_\mu{}^* \alpha_\mu{}^+ + F^+(t), \tag{3.13}$$

$$\dot{\alpha}_\mu{}^+ = -\gamma \alpha_\mu{}^+ - i g_\mu b^+ \sigma_\mu + \Gamma_\mu{}^+(t), \tag{3.14}$$

$$\dot{\sigma}_\mu = \gamma_{11}(d_0 - \sigma_\mu) + 2i(g_\mu \alpha_\mu b^+ - \text{c.c.}) + \Gamma_{\sigma,\mu}(t). \tag{3.15}$$

We note that for running waves the coupling coefficients g_μ have the form

$$g_\mu{}^* = g \exp(ikx_\mu), \tag{3.16}$$

where g is assumed real.

Note that the field mode amplitude b^+ is supported via a sum of dipole moments

$$\sum_\mu \alpha_\mu{}^+ \exp(ikx_\mu) = S_k{}^+. \tag{3.17}$$

We first determine the oscillating dipole moment from Eq. (3.14) which yields in an elementary way

$$\alpha_\mu{}^+ = -ig_\mu \int_{-\infty}^{t} \exp[-\gamma(t-\tau)](b^+\sigma_\mu)_\tau \, d\tau + \hat{\Gamma}_\mu{}^+(t), \tag{3.18}$$

with

$$\hat{\Gamma}_\mu{}^+(t) = \int_{-\infty}^{t} \exp[-\gamma(t-\tau)] \Gamma_\mu{}^+(\tau) \, d\tau. \tag{3.19}$$

In Eq. (3.18) we have dropped the (damped) solution of the homogeneous part of (3.14), because we will consider the stationary state.

We now make a very important assumption which is not only typical for lasers but also for many other cooperative systems. We assume that the relaxation time of the atomic dipole moment α^+ is much smaller than the relaxation time inherent in the order parameter b^+ as well as in σ_μ. This allows us to take $b^+\sigma_\mu$ out of the integral in Eq. (3.18). By this *adiabatic approximation* we obtain

$$\alpha_\mu^+ = -(ig_\mu/\gamma)b^+\sigma_\mu + \hat{\Gamma}_\mu^+(t). \tag{3.20}$$

Equation (3.20) tells us that the atoms obey instantaneously the order parameter. Inserting (3.20) into (3.13) yields

$$\dot{b}^+ = -\kappa b^+ + (g^2/\gamma)b^+\sum_\mu \sigma_\mu + \hat{F}(t), \tag{3.21}$$

where $\hat{F}$ is now composed of the field contribution F and the atomic noise sources Γ,

$$\hat{F}(t) = F^+(t) + i\sum_\mu g_\mu^*\hat{\Gamma}_\mu^+(t). \tag{3.22}$$

In order to eliminate the dipole moments completely we insert Eq. (3.20) into (3.15). A rather detailed analysis shows that one may safely neglect the fluctuating forces which act on the inversion σ_μ. We therefore obtain immediately

$$\dot{\sigma}_\mu = \gamma_{11}(d_0 - \sigma_\mu) - 4(g^2/\gamma)b^+b\sigma_\mu. \tag{3.23}$$

We now again assume that the atom obeys the field instantaneously, i.e., we put

$$\dot{\sigma}_\mu = 0 \tag{3.24}$$

so that the solution of (3.23) reads

$$\sigma_\mu = d_0/[1 + 4(g^2/\gamma\gamma_{11})b^+b]. \tag{3.25}$$

Because we will later be mainly interested in the threshold region where the characteristic laser features emerge and in that region b^+b is still a small quantity, we replace Eq. (3.25) by the expansion

$$\sigma_\mu = d_0 - 4(g^2/\gamma\gamma_{11})d_0b^+b. \tag{3.26}$$

As we will see immediately, laser action will start at a certain value of the inversion d_0. Because in this case b^+b is a small quantity, we may replace d_0 by d_c in the second term of Eq. (3.26) to the same order of approximation. We introduce the total inversion

$$\sum_\mu \sigma_\mu = D, \tag{3.27}$$

and correspondingly

$$Nd_0 = D_0. \tag{3.28}$$

Inserting (3.26) into (3.21) we obtain [with $Nd_c = (\kappa\gamma/g^2)$]

$$\dot{b}^+ = [-\kappa + (g^2/\gamma)D_0]b^+ - 4(g^2\kappa/\gamma\gamma_{11})b^+bb^+ + \hat{F}(t). \tag{3.29}$$

If for the moment we treat b^+ as a real quantity q, (3.29) is evidently identical with the overdamped anharmonic oscillator discussed in Sec. II, where we may identify

$$[\kappa - (g^2/\gamma)D_0] = a. \tag{3.29a}$$

[compare Eq. (2.12)]. Thus we may apply the results of that discussion in particular to the critical region, where the parameter a changes its sign. We thus find that the concepts of symmetry breaking instability, soft mode, critical fluctuations, critical slowing down, are immediately applicable to the single mode laser and reveal a pronounced analogy between the laser threshold and a (second-order) phase transition.[7]

While we may use the results and concepts exhibited in Sec. II, we may also interpret Eq. (3.29) in the terms of laser theory. If the inversion d_0 is small enough, the coefficient of the linear term of (3.29) is negative. We may safely neglect the nonlinearity, and the field is supported merely by stochastic processes (spontaneous emission noise). Because $\hat{F}$ is Gaussian, b is also given by a Gaussian distribution (for the definition of a Gaussian distribution see Sec. X).

The inverse of the relaxation time of the field amplitude b^+ may be interpreted as the optical linewidth. With increasing inversion d_0 the system becomes more and more undamped. Consequently, the optical linewidth decreases; this is a well observed phenomenon in laser experiments. When a (3.29a) passes through zero, b^+ acquires a new equilibrium position with a stable amplitude. Because b^+ is now to be interpreted as a field amplitude, this means that the light is completely coherent. This coherence is disturbed only by small superimposed amplitude fluctuations caused by $\hat{F}$ and by very small phase fluctuations.[8] Even if we consider (3.29) as an equation for a complex quantity b^+ we may derive the right-hand side from the potential

$$-V(|b|) = [-\kappa + (g^2/\gamma)D_0]|b|^2 - 2(g^2\kappa/\gamma\gamma_{11})|b|^4. \tag{3.30}$$

By methods described in the second chapter, the Fokker–Planck equation can be established and readily solved, yielding[9]

$$f(b) = \mathfrak{N}\exp[-2V(|b|)/Q], \tag{3.31}$$

where $Q = C$ (compare Eq. (2.37)) and measures the strength of the fluctuating forces. The function (3.31) [first derived by Risken (1965) and Lax and Hempstead (1966)] describes the photon distribution of laser light, and has been checked experimentally with great accuracy. [See e.g., Arecchi *et al.* (1967), Arecchi and Schulz–Dubois (1972), Mandel (1969), Pike (1970)].

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[7] These analogies have been found and elaborated by Graham and Haken (1968, 1970), Haken (1970), DeGiorgio and Scully (1970), Goldstein, Scully, and Lee (1971), Grossmann and Richter (1971), Grossman (1973), and Graham (1973).

[8] Note that we have to put $b = r\exp(i\varphi)$, with real amplitude r and phase φ, because b is a complex quantity.

[9] Note a difference in the interpretation of the "variable" b^+, b. In all equations up to (3.29) b^+, b may be interpreted either as classical or quantum mechanical quantities. In (3.30) and (3.31) b must be a classical variable. How one may extract quantum mechanical information from a classical function is explained in Chapter XVI.

So far we have investigated the occurrence of a single coherent wave. Expressing the dipole moments via Eq. (3.20) by the field [using also (3.26)], we may readily calculate the correlation function between the α's. For small inversion we thus find

$$\langle\alpha_\mu^+(t)\alpha_\nu(t')\rangle = (g^2/\gamma^2)\exp[ik(x_\mu - x_\nu)]d_0^2\langle b^+(t)b(t')\rangle. \qquad (3.32)$$

Our results up to now may be summarized as follows: If the atomic damping constants γ and γ_{11} are big enough (which is realized in many laser systems), the adiabatic principle applies, which means that the atoms are forced to obey immediately the order parameter. We must now discuss in detail why just one order parameter is dominant. If all parameters would matter simultaneously the system would still be completely random.

E. The multimode laser

We now repeat the preceding steps for the multimode case. We anticipate that the field mode with amplitude b_λ^+ may be decomposed into a rapidly oscillating part with frequency Ω_λ and a slowly varying amplitude B_λ^+:

$$b_\lambda^+ = B_\lambda^+ \exp(i\Omega_\lambda t). \qquad (3.33)$$

The integration of Eq. (3.10) yields

$$\alpha_\mu^+ = -i\sum_\lambda g_{\mu\lambda}\int_{-\infty}^{t}\exp([i\nu - \gamma)(t-\tau)] \times (b_\lambda^+\sigma_\mu)_\tau\, d\tau + \hat{\Gamma}_\mu^+. \qquad (3.34)$$

Using in it (3.33) and making again the adiabatic approximation, we find

$$\alpha_\mu^+ = -i\sum_\lambda g_{\mu\lambda}\{i(\Omega_\lambda - \nu) + \gamma\}^{-1}b_\lambda^+\sigma_\mu + \hat{\Gamma}_\mu^+. \qquad (3.35)$$

We insert (3.35) into (3.9) and use the abbreviation

$$\delta\omega_\lambda = \omega_\lambda - \Omega_\lambda. \qquad (3.36)$$

We thus obtain

$$\exp(i\Omega_\lambda t)\dot{B}_\lambda^+ = i(\delta\omega_\lambda - \kappa_\lambda)b_\lambda^+ + \sum_{\mu\lambda'}\frac{g_{\mu\lambda}^* g_{\mu\lambda'}}{i(\Omega_{\lambda'} - \nu) + \gamma}b_{\lambda'}^+\sigma_\mu + \hat{F}_\lambda. \qquad (3.37)$$

We now consider explicitly the case in which we have a discrete spectrum of modes and we assume further that we may average over the different mode phases, which in many cases is quite a good approximation. (It is also possible, however, to treat phaselocking which is of practical importance for the generation of ultrashort pulses.) Multiplying Eq. (3.37) by b_λ and taking the phase average we have

$$\overline{B_\lambda^+ B_{\lambda'}} = n_\lambda\delta_{\lambda\lambda'}, \qquad (3.38)$$

where n_λ is the number of photons of the mode λ. If we neglect for the time being the fluctuating forces in Eq. (3.37), we obtain

$$\dot{n}_\lambda = -2\kappa_\lambda n_\lambda + n_\lambda w_\lambda D, \qquad (3.39)$$

with

$$w_\lambda = 2\gamma g^2/[(\Omega_\lambda - \nu)^2 + \gamma^2], \qquad (3.40)$$

$$|g_{\mu\lambda}|^2 = g^2. \qquad (3.41)$$

In the same approximation we find

$$\dot{\sigma}_\mu = \gamma_{11}(d_0 - \sigma_\mu) - 2\sum_\lambda w_\lambda n_\lambda\sigma_\mu, \qquad (3.42)$$

or after solving (3.42) again adiabatically

$$D \equiv \sum_\mu \sigma_\mu \approx D_0 - (2D_c/\gamma_{11})\sum_\lambda w_\lambda n_\lambda, \qquad (3.43)$$

where D_c is the critical inversion of all atoms at threshold.

We want to show that Eqs. (3.39)–(3.43) lead to the selection of modes (or order parameters). Consider as an example just two modes. Then the time-independent equations (3.39) read

$$n_1(-2\kappa_1 + w_1 D) = 0, \qquad (3.44)$$

$$n_2(-2\kappa_2 + w_2 D) = 0. \qquad (3.45)$$

If both modes would be present, $n_1 \neq 0$, $n_2 \neq 0$. Then necessarily Eqs. (3.44)–(3.45) must be fulfilled, so that

$$D = 2\kappa_1/w_1, \qquad (3.46)$$

and simultaneously

$$D = 2\kappa_2/w_2. \qquad (3.47)$$

In practical lasers, however, the decay constants κ_λ may be different, and the mode frequencies Ω_λ have different distances from the line center ν. Thus in general (3.46) $\neq$ (3.47). This contradiction can only be resolved if only one mode is present and the other one has died out. This analysis can also be done quite rigorously for many modes and shows that in the laser system only a single mode, the one with the smallest losses and closest to resonance survives. All the others die out. It is worth mentioning that equations of the type (3.39), (3.43) have been proposed more recently in order to develop a mathematical model for evolution [Eigen (1971)]. We will come back to this point in Sec. VI.

As we have seen in Sec. II it is most desirable to establish the Fokker–Planck equation and its stationary solution because it gives us the over-all picture of global and local stability and the size of fluctuations. The solution of the Fokker–Planck equation which is associated with Eqs. (3.37)–(3.43) has been found and reads [compare Haken (1969a)]

$$f(B_\lambda) = \mathfrak{N}\exp(-2\phi/Q), \qquad (3.48)$$

where

$$2\phi = \sum_{\lambda} | B_\lambda |^2 (2\kappa_\lambda - w_\lambda D_0) + (2D_c/\gamma_{11}) \times \sum_{\lambda\lambda'} w_\lambda w_{\lambda'} | B_\lambda |^2 | B_{\lambda'} |^2. \tag{3.49}$$

The local minima of ϕ describe stable or metastable states. This solution allows us to study multimode configurations if some modes are degenerate.

F. Laser with continuously many modes

The next example which is slightly more involved will allow us to make contact with the Ginzburg–Landau theory of superconductivity. Here we assume a *continuum of modes* all running in one direction. As in the case just considered we expect that only modes near resonance will have a chance to participate in laser action, but because the modes are now continuously spaced we must take into consideration a whole set of modes near the vicinity of resonance. Therefore we expect (this must be proven in a self-consistent way) that only modes with

$$| \Omega_\lambda - \nu | \ll \gamma \tag{3.50}$$

and

$$| \Omega_\lambda - \Omega_{\lambda'} | \ll \gamma_{11} \tag{3.51}$$

are important near laser threshold. Inserting Eq. (3.35) into Eq. (3.11) we obtain

$$\dot{\sigma}_\mu = \gamma_{11}(d_0 - \sigma_\mu) - 2\sigma_\mu \sum_{\lambda\lambda'} \left(\frac{g_{\mu\lambda} g_{\mu\lambda'}^*}{i(\Omega_{\lambda'} - \nu) + \gamma} \times b_\lambda^+ b_{\lambda'} + \text{c.c.} \right) \tag{3.52}$$

which under the just mentioned simplifications reduces to

$$\sigma_\mu \approx \left(d_0 - \frac{2d_c}{\gamma_{11}} \sum_{\lambda\lambda'} \frac{g_{\mu\lambda} g_{\mu\lambda'}^*}{\gamma} b_\lambda^+ b_{\lambda'} + \text{c.c.} \right). \tag{3.53}$$

Inserting this into (3.37) yields

$$\dot{b}_\lambda^+ = \left(i\omega_\lambda - \kappa_\lambda + D_0 \frac{g^2}{i(\Omega_\lambda - \nu) + \gamma} \right) b_\lambda^+ + \hat{F}_\lambda(t) - \frac{4d_c}{\gamma_{11}\gamma^2} \sum_{\mu\lambda'\lambda''\lambda'''} g_{\mu\lambda}^* g_{\mu\lambda'} g_{\mu\lambda''} g_{\mu\lambda'''}^* b_{\lambda'}^+ b_{\lambda''}^+ b_{\lambda'''}. \tag{3.54}$$

Using the form (3.16) one readily establishes

$$\sum_\mu g_{\mu\lambda}^* g_{\mu\lambda'} g_{\mu\lambda''} g_{\mu\lambda'''}^* = N g^4 \delta(k_\lambda - k_{\lambda''} - k_{\lambda'} + k_{\lambda'''}), \tag{3.55}$$

where N is the number of laser atoms. Note that we have again assumed (3.50) in the nonlinear part of (3.54). If

$$\Omega_\lambda = \omega_\lambda + \text{Im} D_0 g^2 / [i(\Omega_\lambda - \nu) + \gamma] \tag{3.56}$$

possesses no dispersion i.e. $\Omega_\lambda \propto k_\lambda$ the following exact solution of the corresponding Fokker–Planck equation holds

$$f(b) = \mathfrak{N}_0 \exp(2\phi/Q), \tag{3.57}$$

where

$$\phi = \sum_\lambda | b_\lambda |^2 \left(D_0 \frac{\gamma g^2}{(\Omega_\lambda - \nu)^2 + \gamma^2} - \kappa_\lambda \right) - \frac{2D_c}{\gamma_{11}\gamma^2} g^4 \times \sum_{\lambda\lambda'\lambda''\lambda'''} \delta(k_\lambda - k_{\lambda''} + k_{\lambda'} - k_{\lambda'''}) b_{\lambda'}^+ b_{\lambda''}^+ b_\lambda b_{\lambda'''}. \tag{3.58}$$

We do not continue the discussion of this problem here in the mode picture but rather establish the announced analogy with the Ginzburg–Landau theory. To this end we assume

$$\omega_\lambda = c \, | k_\lambda |, \tag{3.59}$$

$$\Omega_\lambda = v \, | k_\lambda |, \tag{3.60}$$

$$\kappa_\lambda = \kappa. \tag{3.61}$$

Confining ourselves again to modes close to resonance, we use the expansion

$$\frac{g^2}{i(\Omega_\lambda - \nu) + \gamma} = \frac{g^2}{\gamma} - i \frac{g^2}{\gamma^2} (\Omega_\lambda - \nu) - \frac{g^2}{\gamma^3} (\Omega_\lambda - \nu)^2. \tag{3.62}$$

We now replace the index λ by the wave number k, and form the wave packet

$$\Psi^+(x, t) = \int_{-\infty}^{+\infty} B_k^+ \exp(-ikx + iv \, | k | \, t) \, dk. \tag{3.63}$$

The Fourier transformation of Eq. (3.54) is straightforward and we obtain

$$\dot{\Psi}^+(x, t) = -a\Psi^+(x, t) - c[iv(d/dx) - \nu]^2 \Psi^+(x, t) - 2b \, | \Psi(x, t) |^2 \Psi^+(x, t) + F(x, t), \tag{3.64}$$

where in particular the coefficient a is given by

$$a = [\kappa - (g^2/\gamma) D_0]. \tag{3.65}$$

Equation (3.64) is identical with the equation of the electron–pair wavefunction of the Ginzburg–Landau theory of superconductivity for the one-dimensional case if the following identifications are shown in Table I. Note, however, that our equation holds for systems far from thermal equilibrium where the fluctuating forces, in particular, have quite a different meaning. We may again establish the Fokker–Planck equation and translate the solution (3.57), (3.58) to the continuous case which yields.[10]

$$f = \mathfrak{N}_0 \exp(2\phi/Q), \tag{3.66}$$

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[10] Compare footnote 9 on page 77.

TABLE I. Comparison between superconductors and lasers.

Superconductor	Laser
1. Ψ Pair wavefunction	Electric field strength
2. $a \propto T - T_c$	$a \propto D_c - D$
3. T Temperature	D Total inversion
4. T_c Critical temperature	D_c Critical inversion
5. $\nu \propto A_x$ Component of vector potential	ν Atomic frequency
6. $F(x, t)$ Thermal fluctuations	Fluctuations caused by spontaneous emission etc.

with

$$\phi = \int \{a \mid \Psi(x,t) \mid^2 - b \mid \Psi(x,t) \mid^4 - c \mid [iv(d/dx) - \nu]\Psi^+ \mid^2\} \, dx. \tag{3.67}$$

Equation (3.66) is identical with the expression for the distribution function of the Ginzburg–Landau theory of superconductivity if we identify (in addition to Table I) 2ϕ with the free energy, and Q with k_BT. The analogy between systems away from thermal equilibrium and in thermal equilibrium is so evident that it needs no further discussion. As a consequence, however, methods originally developed for one-dimensional superconductors are now applicable to lasers and vice versa.

In the last section of this section we want to show that in spite of this formal analogy there are still deeply rooted differences in the underlying mechanism. In order not to bore the reader with mathematical details, we present a phenomenological approach, which may be substantiated, however, by a rigorous treatment (compare Sec. XI.C).

G. A phenomenological approach to the single mode laser[11]

As we have seen before, the mode amplitude b^+, the Fourier component of the total atomic polarization P, and the total inversion may serve as suitable macroscopic variables. We now discuss the interplay between these three variables, which in the quantum mechanical domain are represented by operators

mode amplitude: b^+, b with $[b, b^+] = 1$

atomic polarization [compare Eq. (3.17), where we drop the index k]: S^+, S^- with $[S^+, S^-] = 2S_z$

atomic inversion [compare Eq. (3.27)]: $D = 2S_z$ (3.68)

We use a notation which clearly exhibits the analogy to spin systems, where the S's have the usual meaning. Note that the electric polarization is obtained from S^+, S^- by multiplication with a factor, which contains essentially the atomic dipole matrix element. The interaction Hamiltonian may be obtained directly from Eq. (3.8) and reads (we assume exact resonance and work in the interaction representation)

$$H = \hbar g(b^+S^- + bS^+). \tag{3.69}$$

In the following we assume that the interaction between atoms and field is dominant over their individual interaction with the reservoirs. In a first step we consider only Eq. (3.69). It allows for several constants of motion h_j:

the interaction energy	$h_0 = H$
the total number of photons and inverted atoms	$h_1 = b^+b + S_z$
the total pseudo spin	$h_2 = S_z^2 + \frac{1}{2}S^+S^- + \frac{1}{2}S^-S^+$ (3.70)

The third quantity follows from the fact that S^+, S^-, S_z behave like spin operators. We now use the method of quantum-classical correspondence, which we will explain in Part II in more detail. It allows us to establish a one-to-one correspondence between operators and classical quantities such as field amplitudes, classical polarization and the occupation number of atoms. In view of a precise formulation of the conservation laws we now distinguish explicitly between operators and classical variables.

field amplitude	$b, b^+ \leftrightarrow u, u^*$
polarization	$S^-, S^+ \leftrightarrow v, v^*$
inversion	$2S_z \leftrightarrow D$ (3.71)

The integrals of motion may be expressed by the classical quantities as may be shown by detailed calculations

$$h_0 = u^*v + uv^*,$$
$$h_1 = u^*u + D/2,$$
$$h_2 = D^2/4 + v^*v. \tag{3.72}$$

(Note that we have dropped the factor $\hbar g$ in h_0, because it is not needed in our following considerations). Now let us look at the stationary distribution function $f(u, v, D)$ which gives the probability of finding a configuration u, v, D. With no coupling to the external world, all configurations which are compatible with the conservation laws may be realized. Thus the probability of finding a certain configuration of u, v, D will depend on these coordinates via the conservation laws:

$$f = f(h_0(u,v,D), h_1(u,v,D), \cdots), \tag{3.73}$$

where f may be an arbitrary function. In this sense the system is highly degenerate.

Now consider the coupling of the proper laser system of atoms and field to its surroundings ("reservoirs"). Then depending on the temperatures of the reservoirs e.g., certain energies are favored compared to others. In thermal equilibrium, f would thus acquire the Boltzmann distribution function $\sim\exp(-H/kT)$. Similarly we expect that in our more general case f is no longer a completely arbitrary function but will acquire a specific form. If we admit that the system finds a stationary state, we expect that the values of h_0, h_1, h_2 are centered around certain values giving a maximum probability around which the distribution

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[11] We follow essentially Haken (1973b).

function will fall off in a Gaussian way. An example for f would be a product of functions of the form

$$\exp(-\alpha_j(\beta_j - h_j)^2), \tag{3.74}$$

where α_j, β_j are constants.

Let us furthermore assume that the phase of the polarization is heavily damped by its coupling to external heatbaths, such as lattice vibrations etc. We then expect that the constant of motion h_0 is also heavily damped because it depends on the phases of v. Thus we are left only with the distribution function of the two other constants of motion. We further use the fact that the action of the heatbaths on the polarization stems from many statistically independent events, and that the effect of this reservoir is dominant over the other ones. Under these conditions $f \sim \exp(-C\,|\,v\,|^2)$, i.e. a Gaussian distribution in v (C is a parameter). Because, however, v must occur via the constant of motion

$$h_2 = |\,v\,|^2 + D^2/4, \tag{3.75}$$

we expect a distribution function of the form

$$f = \mathfrak{N} \exp(-C(|\,v\,|^2 + D^2/4)) \equiv \mathfrak{N} \exp(-Ch_2). \tag{3.76}$$

The factor $\mathfrak{N}$ may still depend on h_1. Assuming for $\mathfrak{N}$ the form (3.74) as discussed above, we obtain finally

$$f_0 = N_0' \exp(-\alpha_1(\beta_1 - h_1)^2) \exp(-Ch_2) \tag{3.77}$$

or, after a slight rearrangement

$$f_0 = N_0 \exp(Ah_1 - Bh_1^2 - Ch_2) \tag{3.78}$$

which is indeed found by a detailed calculation from first principles.

Equation (3.78) exhibits a strong correlation between photon number and inversion. When we integrate over the inversion and polarization we obtain a distribution function of the form

$$\tilde{f}(n) = \tilde{N}_0 \exp(\tilde{a}n - \tilde{b}n^2) \tag{3.79}$$

($n = |\,u\,|^2$) which we have given in (3.31). Our derivation of (3.79) has revealed, however, that (3.79) is a consequence of the second two conservation laws of (3.72), but not of the first one, which represents the energy. Thus there exists a fundamental difference between the laser and a thermodynamic system showing a phase transition e.g., the superconductor. We conclude with a final remark. In our derivation we did not make assumptions about the decay rates of u and D, which may even be equal, so that our analysis applies also to mode-mode coupling theory. [Note that hitherto Eq. (3.79) could be derived only using an adiabatic elimination of the inversion D].

H. Further instabilities

Let us briefly return to the question of the validity of the adiabatic principle. When the laser is pumped more and more, the relaxation time of the field amplitude becomes shorter and shorter. Thus the adiabatic elimination of the atomic variables is finally no longer permissible. If one keeps all variables, one finds at a high enough pump power a new instability [Graham and Haken (1968b); and particularly Risken and Nummedal (1968)]. The laser starts pulsing or, in other words, shows order in the time domain. This instability may be interpreted as a *hard mode instability*. To our knowledge, so far no analytical treatment of the corresponding stochastic problem exists.

IV. NONLINEAR WAVE INTERACTIONS

In physics there are numerous examples of nonlinear wave interactions, e.g., in plasma physics [see e.g., Klimontovich (1967)], in nonlinear transport in crystals [see e.g. Wagner (1973)], nonlinear optics [see e.g. Bloembergen (1965)] etc. Here we want to sketch a few problems with the following characteristic features:

(1) Dissipation and fluctuation are included.
(2) There exist pronounced transitions from disorder to order.

We take our examples here from nonlinear optics, though a number of them can also be realized by electronic devices [see e.g., Woo and Landauer (1971)]. Consider an electromagnetic wave with frequency ω_0 impinging on a crystal. This wave causes the electronic (or molecular) moments to oscillate. In classical dispersion theory, the crystal is treated as a set of (electronic or molecular) oscillators with a linear restoring force. If the field strength is high enough, the amplitudes of the oscillators become so high that nonlinear terms of the restoring forces are important. These anharmonicities lead to a frequency spectrum of the oscillator, which contains e.g. the frequencies $2\omega_0$ or $3\omega_0$. The oscillator now emits electromagnetic waves with these corresponding frequencies. Thus the incoming wave (ω_0) is transformed into a new one with ($2\omega_0$) or ($3\omega_0$) etc. Admitting for similar combinations of the incoming wave with newly generated ones, a great number of transformations, $\omega_0 \rightarrow \omega'$, can be realized.

In the following we do not explicitly treat the role of the atomic system, which only serves in a sense as catalyser. We consider rather the final effect, which consists in the transformation of the initial wave into a set of new ones. Or in other words: We treat the field modes as the order parameters. This transformation is best described by a Hamiltonian. For this purpose we split the amplitude of a field mode into a time and space-dependent part

$$E_\lambda = E_\lambda(t) u_\lambda(\mathbf{x}). \tag{4.1}$$

We further split $E_\lambda(t)$ into

$$E_\lambda(t) = b_\lambda + b_\lambda^+, \tag{4.2}$$

where

$$b_\lambda \propto \exp(-i\omega_\lambda t); \qquad b_\lambda^+ \propto \exp(+i\omega_\lambda t).$$

In a classical description, b_λ^+, b_λ are time-dependent amplitudes; while in quantum mechanics b_λ^+, b_λ are the well-known creation and annihilation operators of light quanta (we assume u_λ properly normalized).

A typical Hamiltonian then reads

$$\begin{aligned}H &= \hbar\omega_p b_p^+ b_p + \sum_\lambda \hbar\omega_\lambda b_\lambda^+ b_\lambda + \hbar g b_p^+ W(b)\\ &\quad + \hbar g^* b_p W(b^+) + b_p^+ \hbar c \exp(-i\omega_p t)\\ &\quad + b_p \hbar c^* \exp(i\omega_p t). \qquad (4.3)\end{aligned}$$

[For special cases see e.g., Bloembergen (1965), Yariv and Louisell (1966), Louisell (1964)]. The first expression is the energy of the incident "pump" wave, the following sum the energy of the other waves λ (it is understood that from now on λ *does not* comprise p). The terms $\sim g, g^*$ stem from the interaction energy and describe e.g., the annihilation of a quantum p and the simultaneous creation of several other quanta of types λ. We quote a few examples:

subharmonic oscillator

$$W(b) = b_1^2, \qquad \text{with} \quad \omega_p = 2\omega_1 \qquad (4.4)$$

parametric oscillator

$$W(b) = b_1 b_2, \qquad \text{with} \quad \omega_p = \omega_1 + \omega_2 \qquad (4.5)$$

higher order parametric process

$$W(b) = b_1^{n_1} \cdots b_N^{n_N}, \qquad \text{with} \quad \omega_p = n_1\omega_1 + \cdots + n_N\omega_N \qquad (4.6)$$

The last two terms in Eq. (4.3) describe a completely coherent driving force generating the pump wave p.

So far all processes are completely coherent and the problem of a disorder-order transition does not arise. This situation changes immediately, however, when we include damping and fluctuations. We do this in the frame of the equations of motion which in classical and quantum physics have exactly the same form:

$$\begin{aligned}\dot b_p^+ &= (i\omega_p - \kappa_p) b_p^+ + i g^* W(b^+) + i c^* \exp(i\omega_p t)\\ &\quad + F_p^+(t), \qquad (4.7)\\ \dot b_\lambda^+ &= (i\omega_\lambda - \kappa_\lambda) b_\lambda^+ + i g b_p^+ (\partial W/\partial b_\lambda) + F_\lambda^+(t). \qquad (4.8)\end{aligned}$$

These equations must be supplemented by their complex (Hermitian) conjugate counter parts. The terms $-\kappa_p b_p^+$, $-\kappa_\lambda b_\lambda^+$ describe damping of the waves (e.g., by scattering) and $F_p^+(t)$, $F_\lambda^+(t)$ are the fluctuating forces which necessarily accompany dissipation. The physical content of Eqs. (4.7) and (4.8) is this: The coherent driving force (e.g., a laser) $\propto c$ in Eq. (4.7) first generates the pump field p. In Eq. (4.8) the term $\sim b_p^+$ then creates, together with the other b's occurring in $\partial W/\partial b_\lambda$, a field b_λ^+ in a self-consistent way. The b_λ^+'s then react on b_p^+ in (4.7) via $W(b^+)$, leading to a saturation of b_p^+.

A detailed analysis (see also below) reveals the following result: For small external force c, no coherent waves b_λ^+ can be maintained. The fields λ are completely randomly excited so that the statistical average $\langle b_\lambda^+ \rangle = 0$. Above a certain threshold $c = c_{\text{thr}}$, coherent field configurations emerge with stable, nonvanishing amplitudes b_λ^+, as is well known from laser physics. To obtain this result all hitherto known papers [Graham and Haken (1968a), Graham (1968a,b, 1970, 1973a), White and Louisell (1970), Haken (1970d)] proceed as follows:

We first eliminate the main time dependence by replacing

$$\begin{aligned}& b_p^+ \to b_p^+ \exp(i\omega_p t),\\ & b_\lambda^+ \to b_\lambda^+ \exp(i\omega_\lambda t). \qquad (4.9)\end{aligned}$$

We then assume for the damping constants

$$\kappa_p \gg \kappa_\lambda \qquad (4.10)$$

and eliminate the pump adiabatically. From Eq. (4.7) we obtain

$$b_p^+ = (1/\kappa_p)\{ i g^* W(b^+) + i c^* + \tilde F_p^+(t) \} \qquad (4.11)$$

which, inserted into (4.8), yields Langevin equations for the b_λ^+'s, b_λ's alone. Using prescriptions given in Sec. XII, XIII, and XIV one readily establishes the Fokker–Planck equation or in the quantum mechanical case the density matrix equation and subsequently the generalized Fokker–Planck equation, where higher-order derivatives of the distribution function with respect to the variables b_λ^+, b_λ must be neglected. For specialists we note that the Fokker–Planck equation is derived by means of the Wigner distribution function [Graham (1970b, 1973a); Haken (1970d)]. If all κ_λ's are equal

$$\kappa_\lambda = \kappa \qquad (4.12)$$

and W is of one of the forms (4.4), (4.5), (4.6) the application of a theorem described in Chapter XI [Haken (1969a)] allows us to construct the explicit stationary solution, f, immediately. It has the following form [Graham (1970b, 1973b), Haken (1970d), Woo and Landauer (1971)]:

$$f = N \exp(-\phi), \qquad (4.13)$$

where

$$\begin{aligned}\phi &= (2/\kappa\kappa_p)(c^* g W + c g^* W^*) + (2\,|\,g\,|^2/\kappa\kappa_p)\,|\,W\,|^2\\ &\quad + 2\sum_\lambda |\,b_\lambda\,|^2. \qquad (4.14)\end{aligned}$$

(Note that b_λ, b_λ^+ are now complex numbers and no longer operators!)

A still more general class of processes in which several pump fields occur and to which our theorem on page 107 is still applicable has been elaborated by Graham (1973b). Returning to Eq. (4.14) and inserting e.g., (4.4) we obtain [Woo and Landauer (1971)]

$$\begin{aligned}\phi &= (2/\kappa\kappa_p)(c^* g b_1^2 + c g^* b_1^{*2}) + 2\,|\,b_1\,|^2\\ &\quad + (2\,|\,g\,|^2/\kappa\kappa_p)\,|\,b_1\,|^4. \qquad (4.15)\end{aligned}$$

Putting $b = q\exp(i\varphi)$, we find a striking analogy with the model of Chapter II, showing us the applicability of all concepts presented there including again the phase-transition analogy.

In the above example a *coherently* driven pump field is decomposed into new fields showing disorder (incoherence) or order (coherence). Recently examples have been found in which a *completely random pump field* may by the process (4.5) generate a new field with a stable amplitude b_1, i.e., a coherent field. In this case c is put equal to zero, and it is assumed that F_p^+ creates a Gaussian photon distribution in the same way as F_1^+ and F_2^+. Provided the internal coupling constant g is bigger than κ_1, κ_2 (and $\kappa_\lambda \ll \kappa_p$) the photon distribution can be found explicitly (Haken (1974b)). Referring the reader who is interested in further details to that paper, we merely quote the result if the photon numbers n_λ are treated as continuous variables (Haken (1973d)). The distribution function of the generated modes 1 and 2 reads

$$f(n_1, n_2) = N\exp(-\phi), \tag{4.16}$$

where

$$\phi = \frac{n_1}{\overline{n_p}} + \frac{h_1}{\overline{n_2}} + \frac{\kappa_1\overline{n_p}}{\kappa_2\overline{n_2}}\left(1 - \overline{n_1} + \frac{\overline{n_1}}{\overline{n_2}}\right)\ln\left(1 + \frac{h_1}{\overline{n_p}} + \frac{\overline{n_1}}{\overline{n_2}}\right) \tag{4.17}$$

for $h_1 \equiv n_2 - n_1 \geq 0$.

The solution for $h_1 < 0$ may be found by exchanging everywhere the indices 1 and 2. $\overline{n_p}$, $\overline{n_\lambda}$ are the mean thermal photon numbers, due to the coupling of the modes to their respective reservoirs at different temperatures. The integration of Eq. (4.16) over n_2 yields a distribution function $f(n_1)$ which describes the photon statistics of that mode. Provided $\overline{n_1} \ll \overline{n_2}$; $\overline{n_1} \ll \overline{n_p}$ and $\kappa_1 > \kappa_2$ with $\kappa_1, \kappa_2 \ll \kappa_p$, one obtains a pronounced non-Gaussian distribution which comes very close to the photon distribution of the single mode laser (3.31), (3.30). This proves that one may obtain an amplitude stabilized field mode from a completely chaotic pump field.

V. TUNNEL DIODES

The physical properties of active devices using as essential part tunnel diodes as representative components have been treated by Landauer (1961, 1962, 1967, 1971a,b) invoking cooperative phenomena in the spirit of the present article. We will follow Landauer in the main steps of our presentation.

First a brief reminder about tunnel diodes starting with the usual *semiconductor*. A single electron in a semiconductor may be described by a plane wave with wave vector **k** which is modulated by a periodic factor. As is known from quantum mechanical calculations, the corresponding energy levels are grouped in "bands" which are separated by gaps. The simplest case is shown in Fig. 3. If we consider regions in space **x** and in **k** space so that Heisenberg's uncertainty relation $\Delta x \Delta k \gtrsim 1$ is fulfilled, we may simultaneously plot the energy levels as a function of spatial coordinate x (Fig. 3). The ordinate represents the energy of a particle, the abscissa its space coordinate. The energy levels are now filled with electrons of opposite spins according to the Pauli principle.

In a semiconductor at the absolute temperature $T = 0$ the valence band is completely filled and the conduction band completely empty. Doping the semiconductor with *charged impurities* shifts the local potential energy of an electron and consequently the energy bands. If the doping is high enough the energy scheme of the tunnel diode (compare Fig. 4) arises. Because the Fermi level remains constant in the crystal at equilibrium the electrons are now redistributed among the energy levels: we find empty states in the valence band and occupied states in the conduction band. The application of an *external electric field* causes an additional displacement of the energy levels. Depending on the direction of the electric field, we now find the energy schemes of Fig. 5. Clearly, if a small voltage is applied the electrons of the conduction band find free states of the valence band into which they can tunnel. [Note that the concept of tunneling applies also to transitions between energy bands ("Zener tunneling" for the transition valence band → conduction band, "Esaki tunneling" for the transition conduction band → valence band).] If the voltage is increased still further, the number of occupied initial states in the conduction band which can tunnel through to acces-

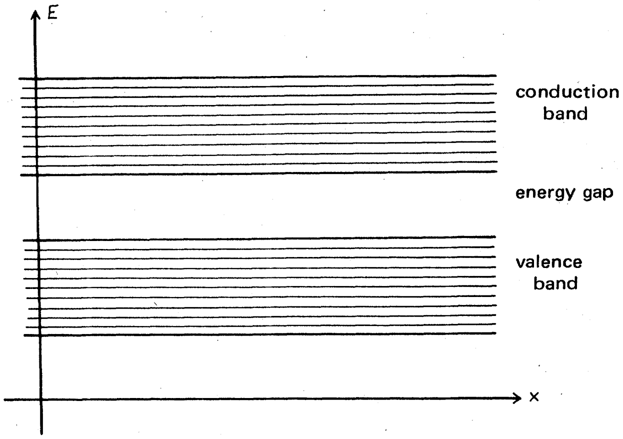

FIG. 3. Energy levels of the energy bands versus coordinate x.

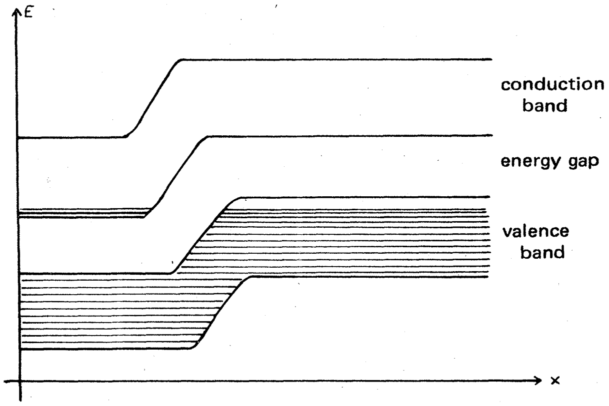

FIG. 4. Occupied and empty energy levels of a tunnel diode (schematic).

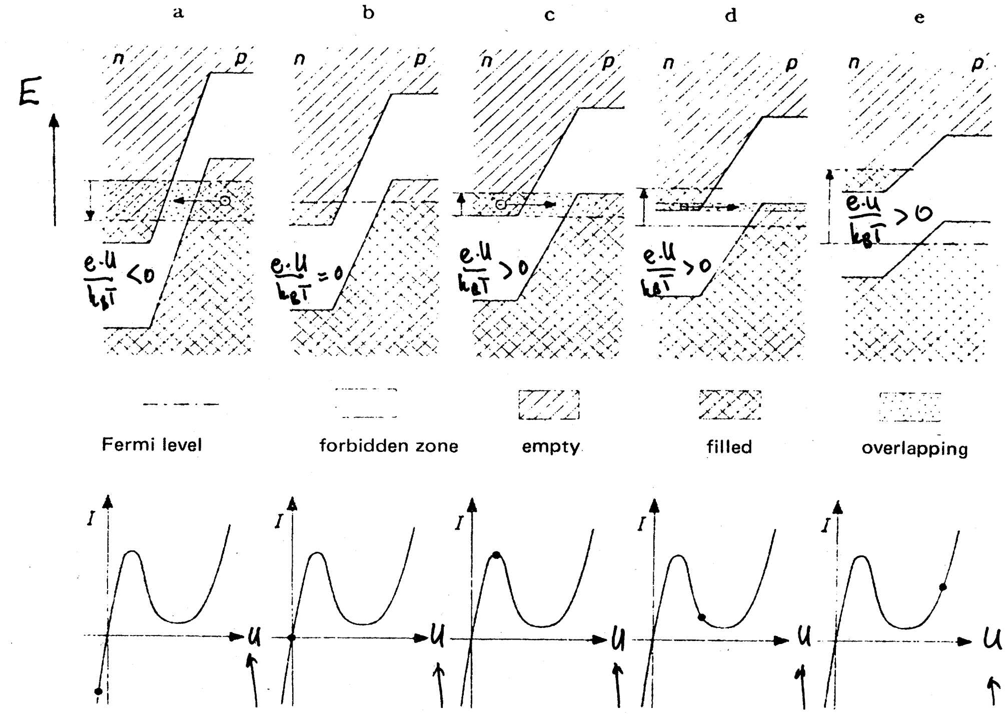

FIG. 5. Energy bands for different voltages and the corresponding points on the characteristic of the tunnel diode.

sible states in the valence band is decreased. Thus the current decreases until finally the situation shown in Fig. 5e is reached. These considerations explain qualitatively the current–voltage relation ("characteristic") of the tunnel diode, represented in Fig. 6 (Landauer (1961). The behavior of a tunnel diode is a typical cooperative effect: Tunneling probabilities depend on voltage and therefore on the number of charges on the capacitance. In this way it is analogous to a ferromagnet in mean field theory, where spin flip probabilities depend on the local field, and therefore on the net magnetization.

We now want to demonstrate, following Landauer, the way in which such tunnel diodes allow us to build circuits in which stable or metastable dissipative states are maintained. Consider as a first example a battery, a tunnel diode and a resistor in series (Fig. 7, Landauer (1962)). In Fig. 6 we present the current voltage characteristic of the tunnel diode again, where V denotes the voltage across the tunnel diode. The voltage across the resistor is then given by

$$V' = V_B - V,$$

where V_B is the voltage of the battery. The current i produced by V' is plotted in Fig. 6, as a function of V for fixed V_B, as a dotted line. If there is a difference between the dotted and the solid line at a given V, we obtain a current flow which charges or discharges the tunnel diode capacitance. In a stationary state the current must vanish so that the crossing points of the solid, and dotted lines give the voltage and current combinations for which we obtain stationary states. Note that these states are maintained by a current, i.e., by an energy flux, so that these states are kept away from thermal equilibrium.

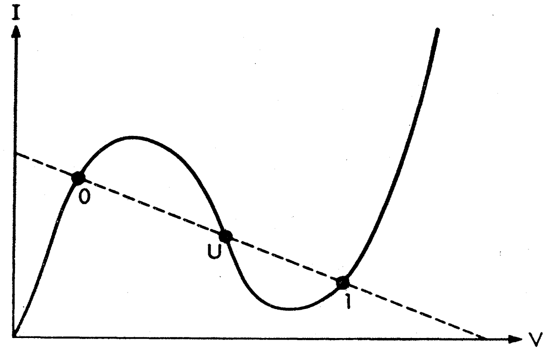

FIG. 6. Negative resistance characteristic (solid line) with load line (dashed). Zero and one are stable states, U is unstable [after Landauer (1961)].

The first most obvious question is this:

(1) Which states are stable, which metastable, which unstable? The answer to this question is of direct technical relevance because we then know in which state we can reliably store information. It will become obvious below, that under certain conditions there are two stable (or metastable) states A'' and C'', which may be identified with "0" and "1" of a computer element.

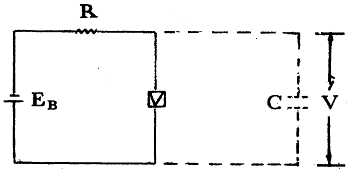

FIG. 7. Tunnel diode fed through series resistance R and diode capacitance C. V is the potential across the diode [after Landauer (1962)].

The next class of questions concerns in a certain sense the reliability of our device:

(2) How probable are voltage (current) fluctuations?

(3) Is there a certain probability the device may go spontaneously from "0" to "1" or vice versa?

(4) How quickly does the system relax to its stable states or leave the unstable state?

Before we demonstrate, following Landauer, how such questions may be answered, we mention that similar considerations may be applied also to devices composed of a battery, a tunnel diode and a thermionic vacuum diode in series or composed of a battery and two tunnel diodes in series. The latter device had been proposed by Goto *et al.* (1960) for switching (bistable elements for computers).

We now proceed to formulate the problem mathematically. A formulation starting from first principles ought to start with the equations of motion of all the electrons of the total device.[12] A much more elegant approach rests on the order parameter concept. We use as order parameter the number N of electrons representing the capacitance charge on the tunnel diode [Landauer (1962)]. To treat the system statistically N is considered as a stochastic variable. Let $n(N)$ be the number of ensemble members with N electrons. Here $n(N)$ changes with time because electrons pass from one side of the tunnel diode to the other or vice versa. We denote the transition rate from a state with N electrons to one with N' electrons by $\Gamma(N,N')$. Because in the limit $dt\to 0$ there is no probability that two or more electrons make a simultaneous transition, the rate equation for $n(N)$ reads[13]

$$\begin{aligned}\partial n(N)/\partial t &= \Gamma(N+1,N)n(N+1)+\Gamma(N-1,N)n(N-1)\\ &\quad-\Gamma(N,N+1)n(N)-\Gamma(N,N-1)n(N). \qquad (5.1)\end{aligned}$$

Though it is not always permissible (as has been stated quite clearly by van Kampen (1961) and Landauer (1962)) to replace the difference Eq. (5.1) by a differential equation,[14] we gain considerable insight into the physical properties by making this approximation (which indeed holds very well at the stationary points). We therefore use the expansion

$$f(N+1)=f(N)+f'(N)+\tfrac{1}{2}f''(N)+\cdots. \qquad (5.2)$$

Because the transition probability multiplied by the charge e has the units of a current we use the abbreviations

$$e\Gamma(N,N-1)=i_D(N) \qquad (D\text{: discharge}), \qquad (5.3)$$

$$e\Gamma(N,N+1)=i_C(N) \qquad (C\text{: charge}). \qquad (5.4)$$

The capacitance charging current is given by the difference between (5.4) and (5.3). For reasons which will become clear below, we write

$$i_C-i_D=\langle\dot{q}\rangle_{\text{av}}, \qquad (5.5)$$

with

$$q=eN, \qquad (5.6)$$

and where $\langle\cdots\rangle_{\text{av}}$ denotes the ensemble average.

We now put

$$f(q)\,dq=N_0 n(N)\,dN, \qquad (5.7)$$

where N_0 is chosen in such a way, that $f(q)$ is normalized to unity and can be interpreted as a probability density. We readily obtain from (5.1) the equation

$$\frac{\partial f}{\partial t}=-\frac{\partial}{\partial q}[(i_C-i_D)f]+\frac{e}{2}\frac{\partial^2}{\partial q^2}[(i_C+i_D)f]. \qquad (5.8)$$

Keeping in mind that i_D, i_c are functions of the charge q [compare Eqs. (5.3), (5.4), (5.6)], Eq. (5.8) has the form of a Fokker–Planck equation where the drift and diffusion coefficients are q dependent.

Let us first discuss the q dependence of the drift coefficient (i_C-i_D) by looking at Fig. 6. Putting $CV=q$, where C is the tunnel diode capacitance, the drift coefficient is just the difference between the currents at charge CV and can be interpreted as a q-dependent force. This force possesses an effective potential in the sense discussed in Sec. II. From the potential we may deduce approximately which states are stable, unstable, and metastable. For a more exact calculation it is, however, necessary to take the q dependence of the diffusion coefficient

$$D=\tfrac{1}{2}e(i_C+i_D) \qquad (5.9)$$

into account, which we will do below. D represents shot noise because (5.3) and (5.4) are transition rates (aside from the factor e) and thus the noise is proportional to the sum of the two uncorrelated currents flowing in opposite directions. We now solve Eq. (5.8). We write (5.8) in the form

$$\partial f/\partial t=-(\partial j/\partial q) \qquad (5.10)$$

and split j up into

$$j=v_q f-D(\partial f/\partial q) \qquad (5.11)$$

with

$$v_q=\langle\dot{q}\rangle_{\text{av}}-(\partial D/\partial q). \qquad (5.12)$$

Note that at other places in this paper, e.g. in (2.33), the right-hand side of the Fokker–Planck equation is split up differently. According to Landauer it is this present form which gives [in the term (5.12)] the motion of ensemble members due to the forces which favor a nonuniform

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[12] Such considerations apply, of course, to any electric network. From a physicist's viewpoint one ought to treat the motion of all electrons of the network. Instead, one introduces macroscopic quantities like currents and charges. In this sense the corresponding equations are "order parameter equations." Furthermore, the microscopic "underground" still manifests itself by fluctuations (noise) of the order parameters. Seen from this point of view, it is perhaps not astonishing that similar concepts apply both to electric networks and to other physical systems.

[13] Carrier density fluctuations have also been treated by Burgess (1950) and others, with different emphasis, however.

[14] It is also possible to solve the difference equation (5.1) exactly (Landauer, 1962). For the general method see Sec. XI.E.

ensemble distribution. $\langle \dot{q} \rangle_{\mathrm{av}}$, without the correction term $-\partial D/\partial q$, also includes terms due to mobility gradients, which arise from the fact that the ensemble member can jump farther from a given point in one direction than the other, but these terms do not correspond toward tendencies for nonuniform equilibrium distribution. For a detailed discussion of the appropriate splitting up of the different terms of the Fokker–Planck equation and their physical interpretation, which is of particular interest for research workers in the field of diffusion, compare Landauer and Woo (1973).

From Eqs. (5.10), (5.11), and (5.12) we find immediately the stationary distribution function. We have only to put

$$j = 0 \tag{5.13}$$

and find explicitly

$$f = f_0 \exp\int (v_q/D)\, dq. \tag{5.14}$$

The negative exponent of (5.14) has, qualitatively, the form of Fig. 1, of Sec. II though it may be asymmetric. Most important, one may change the fictitious potential from the shape of the solid curve to the shape of the dashed curve of Fig. 1 by changing the battery voltage (note that the crossing points A, D, C are shifted by that change!)

A comparison with the considerations of Sec. II shows that all the concepts of phase-transition theory such as symmetry breaking instabilities, soft mode, critical fluctuations etc. become applicable to our device. These and related considerations are fundamental for questions concerning energy consumption, and the reliability of switches (Landauer 1961, 1962, 1967). Here we sketch only some aspects, referring the reader for a detailed treatment to Landauer's papers, and consider the following *switching process*.

Let us assume that we have information stored in the stable state A. Then by continuously changing the fictitious potential V of Fig. 1 (Sec. II) we may eliminate the barrier and then wait until the fluctuations have driven the system into the other states where it remains now locked if the potential is returned to its original form. The information state has changed; C is now occupied. From considerations of this sort one may derive expressions for switching speeds, for error probabilities during switching (probability for remaining in the undesired state) and for the extra energy consumption required by the switching process. The two information states (A, C) are separated by a "barrier" (B). Qualitatively the higher the barrier, the harder the intentional switching becomes. Lowering the barrier spoils the reliability, however, because the information may diffuse more easily from A to C, without external switching. This diffusion process is the second aspect we want to discuss.

Let us assume that we have put the system into the neighborhood of its stable point A. Its distribution function $f_0(q)$ is then centered around $q = q_A$. This critical distribution $f_0(q)$ is, however, by no means the stationary solution (5.14), which has maxima both at A and C. Because $f_0(q)$ develops after a certain relaxation time τ into $f(q)$, we may find the system with practically equal probability (depending on the exact form of f) in both states. The device has lost its information. The determination of τ is thus of fundamental importance. We merely quote Landauer's result (1962)

$$(1/\tau) = (2\pi\tau_B)^{-1}\{\exp(-\Delta A) + \exp(-\Delta C)\}. \tag{5.15}$$

The quantities τ_B, ΔA, ΔB are defined as follows: τ_B is the "relaxation" time, occurring in the linearized Langevin equation near the unstable point $q = q_B$

$$v_q = -(q - q_B)/\tau_B. \tag{5.16}$$

Here τ_B is a measure for how quickly the system leaves B. The "free energies of activation" ΔA and ΔC are defined such that

$$\exp(\Delta A) = N_{SS}(A)/N_{SS}(B) \tag{5.17}$$

and

$$\exp(\Delta C) = N_{SS}(C)/N_{SS}(B). \tag{5.18}$$

Here $N_{SS}(A)$, $N_{SS}(C)$ are the integrated probabilities of finding the system in the wells A or C respectively, whereas $N_{SS}(B)$ is defined by

$$N_{SS}(B) = f(q_B)(2\pi D(q_B)/\tau_B)^{1/2}. \tag{5.19}$$

A closer inspection of Eq. (5.15) reveals that the behavior of τ as a function of the system parameters is governed by an exponential function of the form (5.14). Thus if the potential barrier is increased even only modestly, the system can be efficiently protected against "diffusion."

In conclusion, let us make the following remarks: The present example is to our knowledge the first in which the analogy between the distribution function of a system away from thermal equilibrium and the Boltzmann distribution function was discovered (Landauer 1962, 1971a,b, 1972). To demonstrate this analogy we rederive (5.14) in a formal manner.[15] The Boltzmann distribution would be given by

$$f(q) \propto \exp(-V/kT), \tag{5.20}$$

where the potential energy V can be obtained in a formal way by integration

$$\exp\left(-\int^q \frac{1}{k_B T}\frac{dV}{dq}\,dq\right). \tag{5.21}$$

Multiplying numerator and denominator by the particle mobility μ we obtain

$$\exp\left(-\int^q \frac{1}{\mu k_B T}\cdot\mu\frac{dV}{dq}\,dq\right). \tag{5.22}$$

When we are dealing with the Brownian motion of a particle with the mobility μ we know that the numerator under the integral in (5.22) is just the particle velocity q, whereas the denominator $\mu k_B T$ is the diffusion constant D. Now we may

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[15] Landauer, in his original papers, went the other way, showing that the Boltzmann distribution is a special case of Eq. (5.14).

immediately identify the resulting expression

$$\exp\left(-\int^{q}\frac{\dot{q}\,dq}{D}\right) \tag{5.23}$$

with Eq. (5.14). Though it was possible by a formal analogy to deduce (5.14) from (5.20) an important difference should be noted. Equation (5.14) is much more general because D need not depend on the temperature, as in the case of Brownian motion, and furthermore it can be a complicated function of q.

VI. COOPERATIVE EFFECTS IN CHEMICAL REACTIONS

Because chemical reactions take place between several varieties of molecules, there exists an interaction in a rather trivial sense. What we have in mind, however, is a more sophisticated cooperative effect which leads e.g., to instabilities of the chemical reaction and even in some cases to oscillatory behavior. As order parameters for such chemical reactions we may take the concentrations of molecules which may depend on space and time. This implies that we are dealing with some sort of local equilibrium, which has been pointed out and investigated in detail by Prigogine and coworkers (see e.g. Glansdorff and Prigogine (1971)). As we have seen in many instances cited in the present article one may either consider equations for the mean value of the concentrations ("rate equations"), or an equation for the distribution function allowing also for fluctuations ("stochastic equations"). Here we want to treat two simple examples illustrating these two approaches.

A. Rate equation approach

1. Competition and selection of molecule production

We first consider the following *autocatalytic reaction*: Molecules of type X are generated from molecules of type A by the autocatalytic action of molecules X, so that

$$\mathrm{A} + \mathrm{X} \xrightarrow{k} 2\mathrm{X}, \tag{6.1}$$

where k is the corresponding rate constant. We further assume that by action of molecules B the molecules X are decomposed to form molecules C with the rate constant k'

$$\mathrm{X} + \mathrm{B} \xrightarrow{k'} \mathrm{C}. \tag{6.2}$$

We denote the concentration of molecules X by n, those of A and B by n_A, n_B, respectively. The temporal change of the concentration of molecules of type X is then given by

$$\dot{n} = kn_An - k'n_Bn. \tag{6.3}$$

We now consider the case in which there is only a limited supply of molecules of type A, because by each production of an additional X molecule an A molecule is consumed. We thus adopt the relation

$$n_A = n_0 - n, \tag{6.4}$$

where n_0 is the initial concentration of atoms A. Inserting Eq. (6.4) into (6.3), we obtain

$$\dot{n} = (\alpha - \gamma)n - \beta n^2 \tag{6.5}$$

with the constants

$$\left.\begin{aligned} \alpha &= kn_0 \\ \gamma &= k'n_B \end{aligned}\right\}, \tag{6.6}$$

$$\beta = k. \tag{6.7}$$

An equation of type (6.5) is well known from the single mode laser (compare Sec. III). For $\alpha < \gamma$, i.e., for the production rate smaller than the loss rate, there is no production of molecules X. On the other hand, in the opposite case there is at first an exponentially increasing number of molecules X, but due to the nonlinear term a stable state is finally reached which is caused by the limited "food" supply. This kind of equation can be generalized to several types of molecules X_j which again are all created from the same initial substance A. The rate equation then reads[16]

$$\dot{n}_j = k_jn_An_j - \gamma_jn_j, \tag{6.8}$$

where the production rate depends on n_A which has for instance the form

$$n_A = n_0 - \sum_{l=1}^{\mathrm{N}} n_j. \tag{6.9}$$

One may easily show that equations of the type (6.8) with (6.9) lead to the selection of molecules of a certain type, namely those, which have the highest gain coefficient k_j and the lowest loss coefficient γ_j. Actually the same equations hold for certain types of laser modes (compare Chapter III) where n_j denotes the photon number of those modes. In this latter case mode selection has been studied in detail. In this context, it had been suggested [Haken (1971, 1973)] that laser-type equations may be applicable even to certain types of biological processes. This is indeed the basis of Eigen's theory of evolution of biological macromolecules [Eigen (1971)], though from the mathematical point of view he starts with Prigogine's formulation. In order to proceed from selection to evolution it is necessary, exactly as in the laser case, to include spontaneous production of molecules where spontaneous means without autocatalytic action. Denoting the spontaneous production rate by p_j the equation then reads

$$\dot{n}_j = k_jn_An_j - \gamma_jn_j + p_j(t). \tag{6.10}$$

They are in complete formal analogy to laser equations and allow for instance the study of phase transition-like behavior, e.g. the occurrence of a macroscopic occupation number. The basis difference between the laser and the process of evolution is that laser modes form a closed system, whereas by spontaneous production of new molecules (i.e. by *mutation*) new species are continually fed into the total

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[16] Rate equations of this and related types occur also in population dynamics (see, for example, Goel *et al.*, 1971; Montroll, 1972).

system. These new molecules compete with each other and with the old ones again undergoing a selection process.

2. Oscillations and spatial structures

Clearly enough, passing on to more complicated reactions leads us to deal with rate equations of the general form

$$\dot{n}_j = F_j(n_1, \cdots, n_N). \tag{6.11}$$

Such coupled differential equations which are in general nonlinear allow for a variety of solutions including self-sustained oscillations with small or even large amplitudes.[17] We mention as an explicit example the following autocatalytic model which has been studied in detail by the Brussels group: [Lefever and Nicolis (1971), Lavenda *et al.* (1971)].

$$\begin{aligned} &A \rightarrow X, \\ &B + X \rightarrow Y + D, \\ &2X + Y \rightarrow 3X, \\ &X \rightarrow E. \end{aligned} \tag{6.12}$$

The inverse reaction rates are neglected and the initial and final product concentrations A, B, D, E are maintained time independent throughout the system.

Normalizing the concentrations n_j so that the rate constants become unity the rate equations for the intermediate products read

$$\dot{n}_X = n_A - (n_B + 1)n_X + n_X{}^2 n_Y \tag{6.13}$$

$$\dot{n}_Y = n_B n_X - n_X{}^2 n_Y. \tag{6.14}$$

For certain values of n_j ($j = A, B$) a limit cycle may bifurcate from the steady state. Such models thus allow for an understanding of chemical and perhaps even for biological clocks.[18] Taking into account matter transport by diffusion or convection we may generalize equations (6.11) by inclusion of spatial derivatives. In the case of the model (6.12), diffusion was introduced by adding terms

$$D_X(d^2/dx^2)n_X, \qquad D_Y(d^2/dx^2)n_Y$$

to Eqs. (6.13) and (6.14), respectively. (Prigogine and and Lefever (1968), Lefever (1968), Herschkowitz-Kaufman and Nicolis (1972)). Among the different types of solution chemical waves seem to be extremely interesting, particularly with respect to biological processes. Furthermore spatially inhomogeneous solutions may occur. Experimentally, striking wave-propagation phenomena of chemical reactions, including rotating reactions, have been found more recently (Zaikin and Zhabotinsky (1970), (1973); Winfree (1973)). Clearly enough the rate equations e.g., of type (6.10) refer to mean numbers, saying nothing about fluctuations. We finally show by means of a simple example how fluctuations may be taken into account.

B. Stochastic equations (master equation treatment)

We assume the autocatalytic production of molecules of type X from the basic substance A but now take the number of molecules of substance A to be much greater than those of substance X and thus neglect saturation.[19] Instead we assume a bimolecular decay process. Furthermore we allow for a spontaneous production from the original material and consider the final decay of this molecule. Thus this process reads

$$\begin{aligned} &A + X \underset{k_2}{\overset{k_1}{\rightleftarrows}} 2X, \\ &A \overset{k_3}{\rightarrow} X, \\ &X + B \overset{k_4}{\rightarrow} C. \end{aligned} \tag{6.15}$$

It is a simple matter to derive the master equation for the distribution function f of the number of molecules of type X (we assume $k_3 = k_1$)

$$\begin{aligned} &df(n,t)/dt \\ &\quad = \alpha\{nf(n-1) - (n+1)f(n)\}, \\ &\quad + \beta\{n(n+1)f(n+1) - n(n-1)f(n)\}, \\ &\quad + \gamma\{(n+1)f(n+1) - nf(n)\}, \end{aligned} \tag{6.16}$$

where

$$\begin{aligned} \alpha &= k_1 n_A, \\ \beta &= k_2, \\ \gamma &= k_4 n_B. \end{aligned} \tag{6.17}$$

We briefly indicate how to obtain an equation for the mean number which is defined by

$$\bar{n} = \sum_{n=0}^{\infty} nf(n). \tag{6.18}$$

Multiplying (6.16) by n and summing up over n we obtain

$$d\bar{n}/dt = \alpha(\bar{n} + 1) - \gamma\bar{n} - \beta(n^2 - \bar{n}). \tag{6.19}$$

If the fluctuations of n around the mean value are small we may put

$$\overline{n^2} \approx \bar{n}^2. \tag{6.20}$$

Finally neglecting 1 compared to $\bar{n}$ we obtain

$$d\bar{n}/dt = (\alpha - \gamma)\bar{n} - \beta\bar{n}^2 \tag{6.21}$$

which is of the form of Eq. (6.5) discussed above.

Equations of the type (6.16) have been found and discussed e.g., in the section concerning tunnel diodes. Applying Landauer's method of solution (compare also Sec. XI.E)

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[17] The first mathematical model was given by Lotka (1920).

[18] Chemical oscillations have been found in the laboratory, e.g., by Bray (1921), Belousov (1959), and Zhabotinskij (1964), and are at present being studied very intensely.

[19] We follow essentially the paper by K. J. McNeil and D. F. Walls (1974). A related problem (the Lotka–Volterra problem) has been treated by Nicolis (1972).

the stationary solution is found to be

$$f(n) = f(0)(\alpha/\gamma)^n \prod_{l=1}^{n} (1+\mu l)^{-1}, \tag{6.22}$$

with

$$\mu = \beta/\gamma, \tag{6.23}$$

and $f(0)$ is determined by the normalization condition yielding

$$f(0) = \{{}_1f_1(1; 1+1/\mu; \alpha/\beta)\}^{-1}, \tag{6.24}$$

where ${}_1f_1$ is a hypergeometric function. The mean number of molecules is given by

$$\bar{n} = f(0)(\alpha/\gamma)(1+\mu)^{-1}{}_1f_1(2; 2+1/\mu; \alpha/\beta). \tag{6.25}$$

Plotting $\bar{n}$ as a function of the "pump parameter" α one observes a sudden increase of the molecule number above a certain threshold value quite in analogy to the laser, which is no surprise because the underlying equations are practically the same.

It is remarkable that the system above threshold describes a state of higher order which may be proved by looking at the entropy. We define the entropy without further discussion by

$$S = -\sum_{n=0}^{\infty} f(n) \log f(n). \tag{6.26}$$

The evaluation of (6.26) by means of (6.22) yields, somewhat below threshold,

$$S \approx -\frac{\alpha}{\gamma}\log\frac{\alpha}{\gamma} - \log(1-\alpha/\gamma). \tag{6.27}$$

This is identical with the maximum entropy, which is found by the variation of (6.26) under the constraint that $f(n)$ is normalized and the mean number $\bar{n}$ is kept fixed. Somewhat above threshold, however, one finds, again using (6.22),

$$S \approx \tfrac{1}{2}[\log(2\pi(\alpha/\beta)) + 1]. \tag{6.28}$$

Though the entropy is an increasing function of the pump parameter, Eq. (6.28) does not represent the maximum value (6.26) can acquire for a given mean number $\bar{n}$.

Our above remarks, of course, do not exhaust this vast field and we feel that here in particular we are just at a beginning.

VII. INSTABILITIES IN FLUID DYNAMICS[20]

A. The Bénard and Taylor problems

We shall now discuss a set of problems which have fascinated physicists for at least a century because they are striking examples showing how thermal equilibrium states, characterized by complete disorder, may suddenly show pronounced order if one goes away from thermal equilibrium. We shall select the so-called Bénard and Taylor problems.[21]

We first describe the Bénard problem, or, using another expression for it, the convection instability: Let us consider an infinitely extended horizontal fluid layer which is heated from below so that a temperature gradient is maintained. This gradient, if expressed in suitable dimensionless units, is called the Rayleigh number R. As long as the Rayleigh number is not too large, the fluid remains quiescent and heat is transported by conduction. If it exceeds a certain value, however, suddenly the fluid starts to convect. What is most surprising is that the convection pattern is very regular and may either show rolls or hexagons.

The hexagons depicted in Fig. 8 are the convection cells as seen from above. One may have the fluid rising in the middle of the cell and going down at the boundaries or vice versa. An obvious task for a theoretical treatment is to explain the mechanism of this sudden disorder-order transition and to predict the form and stability of the cells. In a more refined theory one may then ask questions as to the probability of fluctuations.

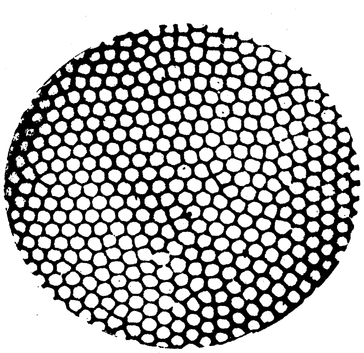

FIG. 8. Bénard cells in spermaceti. A reproduction of one of Bénard's original photographs.

A closely related problem is the so-called Taylor problem: the flow between a long stationary outer cylinder and a concentric rotating inner cylinder takes place along circular streamlines (couette flow) if a suitable dimensionless measure of the inner rotation speed (the Taylor number) is small enough. But Taylor vortices spaced periodically in the axial direction appear when the Taylor number exceeds a critical value.

In the following we treat explicitly the Bénard instability. The physical quantities we have to deal with are the velocity field with components u_j ($j = 1, 2, 3 \leftrightarrow x, y, z$) at space point x, y, z, the pressure p, and the temperature T. Before going to the mathematical details, the situation is described: the velocity field, the pressure, and the temperature obey certain nonlinear equations of fluid dynamics which may be brought into a form depending on the Rayleigh number R which is a prescribed quantity. For small values of R one obtains a solution by putting the velocity components equal to zero. The *stability* of this solution is proven by linearizing the total equations around the stationary values of u, p, T,

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[20] There exists an enormous literature on instabilities and also on fluctuations (including the problem of turbulence) in fluid dynamics. It is not the purpose of this chapter to review this field. We have rather chosen an example which shows striking similarities with the laser instability and which, incidentally, demonstrates clearly the interplay between "coherent" forces and fluctuations.

[21] For a detailed review see, e.g., the book by Chandrasekhar (1968).

where one obtains *damped waves*. If, however, the Rayleigh number exceeds a certain critical value R_c, the solutions become unstable. The procedure is now rather similar to the one which we have encountered in laser theory (compare Sec. III). The solutions which become unstable define a set of modes. We expand the actual field (u, T) into these modes with unknown amplitudes. Taking into account the nonlinearities of the system we now obtain nonlinear equations for the mode amplitudes which quite closely resemble those of laser theory leading to certain stable mode configurations. If we include thermal fluctuations we again end up with a problem defined by nonlinear deterministic forces and fluctuating forces quite in the spirit of Sec. II. Their interplay governs in particular the transition region, $R \approx R_c$.

B. Mathematical treatment

1. The basic equations and the boundary conditions[22]

We start with the so-called Boussinesq approximation from which the equations of fluid mechanics acquire the following form: The *continuity equation* reads

$$\partial u_j/\partial x_j = 0. \tag{7.1}$$

Here and in the following, double indices imply summation over these indices. The equation of *fluid motion* reads

$$\frac{\partial u_j}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} - \frac{1}{\rho_0}\frac{\partial p}{\partial x_i} + (1 + \delta\rho/\rho_0)X_i + \nu\nabla^2 u_i + F_i^{(u)}(x, t). \tag{7.2}$$

Here ρ_0 is the mean density of the fluid, $\delta\rho$ is the deviation from the mean density due to thermal expansion (with the expansion coefficient α)

$$\delta\rho = -\rho_0\alpha(T - T_0). \tag{7.3}$$

X_i are the components of external forces, in our case the gravitation field $\mathbf{X} = (0, 0, -g)$, $\nu = \mu/\rho_0$ is the kinematic viscosity, and μ is the coefficient of viscosity. The fluctuating force $F_i^{(u)}$ has been added to the usual Boussinesq equation.[23] Finally the *equation for the heat conduction* reads

$$\partial T/\partial t = -u_j(\partial T/\partial x_j) + \kappa\nabla^2 T + F^{(T)}(x, t), \tag{7.4}$$

where κ is the thermometric conductivity. $F^{(T)}$ is again a fluctuating force. The fluctuating forces stem from thermal fluctuations and are as usual connected with the dissipation of the system (compare Sec. XII.A).

In the following we adopt Landau's point of view and assume that the fluctuating forces are δ correlated in space and time, but that $F^{(u)}$ and $F^{(T)}$ are mutually uncorrelated. Before proceeding further we note that the nonlinearities

$$u_j(\partial u_i/\partial x_j) \quad \text{and} \quad u_j(\partial T/\partial x_j) \tag{7.5}$$

stem from the so-called *local description* in fluid dynamics. As is well known, the following relation holds for an arbitrary quantity A (e.g., momentum component, energy, etc.)

$$dA/dt = \partial A/\partial t + \mathbf{u}\nabla A. \tag{7.6}$$

The left-hand side of Eq. (7.6) is the rate of change of the quantity A of a fluid particle as it moves in space. The two terms on the right-hand side represent the local change of that quantity A.

Keeping in mind the analogous treatment in laser theory we first consider the stationary state for $R < R_c$ without fluctuating forces. (For the explicit definition of R see (7.20)). In the stationary state there is no fluid motion so that

$$u_j = 0 \tag{7.7}$$

We further put

$$T = T_S = T_0 - \beta z, \tag{7.8}$$

where β is the temperature gradient in the vertical direction needed to describe the spatial dependence of the temperature. With (7.7) and (7.8) one readily fulfills the equations (7.1) and (7.4) (without fluctuating forces:). From Eq. (7.2) one determines the pressure

$$p = p_0 - g\rho_0(z + \tfrac{1}{2}\alpha\beta z^2). \tag{7.9}$$

We now consider the general case including $R \geq R_c$ and transform Eqs. (7.1)–(7.4) further putting

$$T' = T + \Theta. \tag{7.10}$$

The boundary conditions for the quantities $\mathbf{u}$, Θ are as follows. We consider a layer infinite in horizontal extent and the fluid between the planes $z = -(d/2)$ and $z = (d/2)$ For a viscous fluid we have at rigid boundaries

$$u_z = \Theta = 0 \tag{7.11}$$

and at free boundaries

$$u_z = (\partial/\partial z)\epsilon_{izk}u_k = \Theta = 0. \tag{7.12}$$

2. The equations in dimensionless quantities

As usual we proceed to dimensionless quantities defined by

$$\left.\begin{aligned} u_i &= \kappa u_i'/d; \qquad \Theta = \nu\kappa\Theta'/\alpha g d^3, \qquad t = d^2 t'/\kappa \\ x_i &= d x_i', \qquad \bar{\omega} \equiv p/\rho_0 + g(z - \tfrac{1}{2}\beta\alpha z^2) = \kappa^2\bar{\omega}'/d^2 \end{aligned}\right\} \tag{7.13}$$

and

$$F^{(u)} = F^{(u)\prime}\kappa^2/d^3, \tag{7.14}$$

$$F^{(\theta)} = F^{(\theta)\prime}\nu\kappa^2/\alpha d^5 g. \tag{7.15}$$

After dropping the primes from the new variables, our

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[22] See, for example, Chandrasekhar (1968).

[23] Fluctuating forces were introduced into fluid dynamics by Landau (see, for example, Landau and Lifshitz, *Fluid Dynamics*) and used more recently by Zaitsev and Shliomis (1971).

system of equations reads

$$\partial u_j/\partial x_j = 0 \tag{7.16}$$

$$\frac{\partial u_i}{\partial t} = -u_j \frac{\partial u_i}{\partial x_j} - \frac{\partial \tilde{\omega}}{\partial x_i} + P\Theta\lambda_i + P\Delta u_i + F_i^{(u)}, \tag{7.17}$$

$$\lambda = (0, 0, 1)$$

$$\frac{\partial \Theta}{\partial t} = -u_j \frac{\partial \Theta}{\partial x_j} + Ru_z + \Delta\Theta + F^{(\theta)}. \tag{7.18}$$

Here

$$P = \nu/\kappa \tag{7.19}$$

is the Prandtl number and

$$R = \alpha g \beta d^4/\nu\kappa \tag{7.20}$$

the Rayleigh number. If the temperature gradient in z direction varies with time we must replace [Krishnamurti (1968)]

$$Ru_z \tag{7.21}$$

by

$$Ru_z - R\eta' z u_z. \tag{7.22}$$

Here η' is connected with the time-dependent temperature T_S by

$$\eta' = (d^2/\kappa\Delta T)(\partial T_S/\partial t), \tag{7.23}$$

and the boundary conditions now read

$$T_S = \tfrac{1}{2}\Delta T + \eta t \quad \text{at} \quad z = -\tfrac{1}{2}d, \tag{7.24}$$

$$T_S = -\tfrac{1}{2}\Delta T + \eta t \quad \text{at} \quad z = \tfrac{1}{2}d. \tag{7.25}$$

As we will see below such inhomogeneities are necessary in order to explain hexagonal formation.

3. Damped and neutral solutions ($R \leq R_c$)

We treat now Eqs. (7.16)–(7.18) as follows. We first assume that $R < R_c$. Linearizing the nonlinear equations around the values $\mathbf{u} = \Theta = 0$ we obtain, after some calculations, damped solutions

$$\mathbf{u} \sim \exp(-\gamma t); \qquad \gamma > 0 \tag{7.26}$$

We now define the critical value R_c as the one for which γ tends to 0. $R = R_c$ thus defines the marginal (neutral) states. A lengthy but straightforward calculation shows that the neutral solutions may be defined as follows [Schlüter *et al.* (1965)]

$$u_i^{(1)}(\mathbf{x}) = \delta_i v^{(1)}, \tag{7.27}$$

where the operator δ_i is given by

$$\delta_i = (\partial^2/\partial x_i\, \partial z) - \lambda_i \Delta; \qquad \boldsymbol{\lambda} = (0, 0, 1), \tag{7.28}$$

and $v^{(1)}$ by

$$v^{(1)} = w(x, y) g(z). \tag{7.29}$$

The functions w and $g(z)$ are defined as follows: For free boundaries (the origin of the coordinate system is put in the middle of the layer) [see e.g. Pellew and Southwell (1940)]

$$g(z) = (\pi^2 + k^2)^2 \cosh \pi i z = (\pi^2 + k^2)^2 \cos \pi z \tag{7.30}$$

and

$$w(x, y) = \sum_{\mathbf{k}} A_{\mathbf{k}} \exp(i\mathbf{kx}), \tag{7.31}$$

where the coefficients A_k are still arbitrary, and $\mathbf{k}$ lies in the x, y plane,

$$\mathbf{k} = (k_x, k_y), \tag{7.32}$$

having the absolute value

$$k = \pi/\sqrt{2}. \tag{7.33}$$

Without going into all details of the neutral solution we merely mention that the neutral solution may be described by a super-position of formal vectors

$$\overline{\Psi_{\mathbf{k}}} = \begin{pmatrix} \mathbf{u}_{\mathbf{k}}^{(1)} \\ \Theta_{\mathbf{k}}^{(1)} \end{pmatrix}. \tag{7.34}$$

For the following we define the transpose of (7.34) by

$$\Psi_{\mathbf{k}} = (u_{\mathbf{k}}^{(1)}, \Theta_{\mathbf{k}}^{(1)}) \tag{7.35}$$

The $\Theta_{\mathbf{k}}^{(1)}$'s can also be given explicitly.

4. Solution near $R = R_c$ (nonlinear domain) effective Langevin equations

We now expand the velocity field $\mathbf{u}$ (and correspondingly the temperature field) according to Eq. (7.34) into the neutral solutions [compare also Eq. (7.31)]

$$\mathbf{u}(\mathbf{x}) = \sum_{\mathbf{k}} A_{\mathbf{k}} \mathbf{u}_{\mathbf{k}}^{(1)}(\mathbf{x}), \tag{7.36}$$

where the coefficients $A_{\mathbf{k}}$ are still to be determined. We shall even allow the amplitudes $A_{\mathbf{k}}$ to vary slowly with time and space. [Where "slowly means "slowly compared to $\exp(i\mathbf{kx})$".] The main goal is now to establish a set of equations for the coefficients $A_{\mathbf{k}}$ in a region where the Rayleigh number R is different, but still in the vicinity of the critical Rayleigh number R_c. Introducing a small quantity ϵ we define as usual an iteration procedure by [see e.g., Schlüter *et al.* (1965)]

$$\mathbf{u}(\mathbf{x}) = \epsilon \mathbf{u}^{(1)}(\mathbf{x}) + \epsilon^2 \mathbf{u}^{(2)}(\mathbf{x}) + \cdots \tag{7.37}$$

$$\Theta(\mathbf{x}) = \epsilon \Theta^{(1)}(\mathbf{x}) + \epsilon^2 \Theta^{(2)}(\mathbf{x}) + \cdots \tag{7.38}$$

$$R = R^{(0)} + \epsilon R^{(1)} + \epsilon^2 R^{(2)} + \cdots. \tag{7.39}$$

The performance of the iteration procedure is not very difficult but rather lengthy so that we refer the reader to the original literature. We just quote the final result. We put

$$(R - R_c)/R_c = \epsilon^2 \chi \tag{7.40}$$

and use concomitant with Eqs. (7.37)–(7.39) the scaling (Newell and Whitehead (1969)).

$$\tilde{t} = \epsilon^2 t, \qquad X = \epsilon x, \qquad Y = (\epsilon)^{1/2} y. \tag{7.41}$$

In the final equation we then formally put $\epsilon = 1$, and replace X, Y by x, y. By neglecting the additional terms described by Eq. (7.22) etc. we find the following set of equations

$$\begin{aligned}\frac{\partial A_{\mathbf{k}}}{\partial t} &\\ &= \gamma \left(\frac{\partial}{\partial x_{(\mathbf{k})}} - \frac{i}{\sqrt{2}\pi} \frac{\partial^2}{\partial y_{(\mathbf{k})}{}^2} \right)^2 A_{\mathbf{k}} + \alpha A_{\mathbf{k}} \\ &\quad - \sum_{\mathbf{k}'} \beta_{\mathbf{k}\mathbf{k}'} \mid A_{\mathbf{k}'} \mid^2 A_{\mathbf{k}} + F_{\mathbf{k}}(x, y, t)\end{aligned} \tag{7.42}$$

which has the form of Langevin equations for the $A_{\mathbf{k}}$'s. The only thing we have to do beyond the hitherto known procedure is to repeat all the necessary steps including the fluctuating forces [Haken (1973f)]. They are found as projections of the original fluctuating forces on the neutral solutions i.e., as follows:

$$F_{\mathbf{k}}(x, y, t) = \left\langle \left(\overline{\Psi_{\mathbf{k}}}, \begin{pmatrix} F^{(u)} \\ F^{(T)} \end{pmatrix} \right) \right\rangle . \tag{7.43}$$

The brackets $\langle \quad \rangle$ denote an average over the space coordinates over a region large compared to $1/|k|$, but small compared to the wavelength of the resulting fluctuations of $A_{\mathbf{k}}$.

From this definition one readily derives the following correlation functions:

$$\begin{aligned}&\langle\langle F_{\mathbf{k}}(x, y, t) F_{\mathbf{k}'}(x', y', t') \rangle\rangle \\ &\quad = \delta_{\mathbf{k}\mathbf{k}'} \delta(x - x') \delta(y - y') \delta(t - t') Q.\end{aligned} \tag{7.44}$$

The double brackets $\langle\langle \cdots \rangle\rangle$ denote the statistical average over the thermal fluctuations. We obtain

$$Q = \frac{\pi^2 P^2}{4(1 + P)^2} \left[\frac{P^2 \nu k_B \cdot T}{R_c \kappa^3 \cdot d \cdot \rho_0} + \frac{d^3 \cdot g^2 \cdot k_B T^2}{\nu^2 \kappa^2 \rho_0 c_v} \right] \tag{7.45}$$

i.e., the strength Q of the fluctuating forces has the form

$$Q = C_1 T + C_2 T^2. \tag{7.46}$$

The coefficients α, β, γ in Eq. (7.42) are defined as follows:

$$\tilde{\gamma} = 4P/(P + 1), \tag{7.47}$$

$$\tilde{\alpha} = [3P\pi^2/2(P + 1)] \cdot [(R - R_c)/R_c], \tag{7.48}$$

$$\tilde{\beta} = P/2(P + 1), \tag{7.49}$$

where P is the Prandtl number introduced by Eq. (7.19). $\partial/\partial x_{(\mathbf{k})}$ is the derivative in the direction of the $\mathbf{k}$ vector occurring in $A_{\mathbf{k}}$, $y_{(\mathbf{k})}$ the derivative perpendicular to it. We further have

$$\beta_{\mathbf{k}\mathbf{k}'} = \tilde{\beta} \qquad \text{for} \quad \mathbf{k} = \mathbf{k}', \tag{7.50}$$

and put

$$\beta_{\mathbf{k}\mathbf{k}'} = \tilde{\beta}(1 + \beta_{ij}) \qquad \text{for} \quad \mathbf{k} \neq \mathbf{k}'. \tag{7.51}$$

For the following discussion the explicit form of β_{ij} is not very important. We only note that all β_{ij} are positive. If the inhomogeneity described by Eq. (7.22) is taken into account an additional term of the form

$$-\delta \sum_{\mathbf{k}_1, \mathbf{k}_2} A_{\mathbf{k}_1}{}^* A_{\mathbf{k}_2}{}^* \delta_{\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}, 0} \tag{7.52}$$

must be added to the right-hand side of Eq. (7.42) where $\delta \propto \eta'$. [For the sake of completeness we mention that the inclusion of Eq. (7.22) requires a "renormalization" of R_c, k and an altered function $g(z)$ in (7.29). Because this does not change the structure of our following equations, we suppress a detailed discussion here].

An equation of the form (7.42) is now well known to us. We know it already from the chapter on laser theory and we can exploit the methods of solution which have been described there. Before doing so we write (7.42) [if necessary under inclusion of (7.52)] in the form

$$\partial A_{\mathbf{k}}/\partial t = \tilde{L} A_{\mathbf{k}} + N_{\mathbf{k}}(\{A\}) + F_{\mathbf{k}}, \tag{7.53}$$

where L is the linear operator occurring on the right-hand side of Eq. (7.42), whereas $N_{\mathbf{k}}$ contains all the nonlinear terms of that equation.

5. The Fokker-Planck equation and its stationary solution

It is now a simple matter to establish the corresponding Fokker–Planck equation which reads

$$\begin{aligned}\frac{df}{dt} = &- \iint dx\, dy \sum_{\mathbf{k}} \left\{ \frac{\delta}{\delta A_{\mathbf{k}}(x, y)} (\tilde{L} A_{\mathbf{k}}(x, y) \right. \\ &\left. + N_{\mathbf{k}}(\{A(x, y)\})) + \text{c.c.} \right\} f \\ &+ Q \iint dx\, dy \sum_{\mathbf{k}} \frac{\delta^2}{\delta A_{\mathbf{k}}(x, y) \delta A_{\mathbf{k}}{}^*(x, y)} f .\end{aligned} \tag{7.54}$$

We seek its stationary solution in the form

$$f = N \exp \phi \tag{7.55}$$

One readily establishes that the conditions allowing an explicit stationary solution of (7.54) (compare Sec. XI.D) are fulfilled. From it one derives the following explicit solution

$$\phi = \frac{2}{Q}\iint\Big\{\sum_{\mathbf{k}}\gamma A_{\mathbf{k}}^{*}\Big(\frac{\partial}{\partial x_{(k)}}-\frac{i}{2^{1/2}\pi}\frac{\partial^{2}}{\partial y_{(k)}{}^{2}}\Big)^{2}A_{\mathbf{k}}$$
$$+\sum_{\mathbf{k}}\tilde{\alpha}\,|\,A_{\mathbf{k}}\,|^{2}-\tfrac{1}{3}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}(\delta A_{\mathbf{k}_1}{}^{*}A_{\mathbf{k}_2}{}^{*}A_{\mathbf{k}_3}{}^{*}\delta_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3,0}+\text{c.c.})$$
$$-\tfrac{1}{2}\sum_{\mathbf{k}\mathbf{k}'}\beta_{\mathbf{k}\mathbf{k}'}\,|\,A_{\mathbf{k}}\,|^{2}\,|\,A_{\mathbf{k}'}\,|^{2}\Big\}\,dx\,dy. \tag{7.56}$$

(Haken (1973f)); for the special case of a single mode see also Graham (1973b). In Eq. (7.56) we have included terms stemming from (7.52).

6. Stable mode configuration

It goes, of course, far beyond the present article to treat Eq. (7.56) in its whole generality. We want to demonstrate, how such an expression (7.55) and (7.56) allows us to discuss the threshold region and the stability of various mode configurations. We neglect the dependence of the slowly varying amplitudes $A_{\mathbf{k}}$ on x, y. We further put $\delta = 0$. Equations (7.55) and (7.56) give us a suitable means for the discussion of the stability of different mode configurations. Because ϕ depends only on the absolute values of $A_{\mathbf{k}}$

$$\phi = \phi(|\,A_{\mathbf{k}}\,|^{2}) \tag{7.57}$$

we introduce the new variable

$$|\,A_{\mathbf{k}}\,|^{2} = w_{\mathbf{k}}. \tag{7.58}$$

The values $w_{\mathbf{k}}$ for which ϕ has an extremum are given by

$$\frac{\partial\phi}{\partial w_{\mathbf{k}}} = 0, \qquad \text{or} \qquad \tilde{\alpha}-\sum_{\mathbf{k}'}\beta_{\mathbf{k}\mathbf{k}'}w_{\mathbf{k}'} = 0, \tag{7.59}$$

and the second derivative tells us that the extrema are all maxima

$$\partial^{2}\phi/\partial w_{\mathbf{k}}\,\partial w_{\mathbf{k}'} = -\beta_{\mathbf{k}\mathbf{k}'} < 0. \qquad \text{maximum} \tag{7.60}$$

For symmetry reasons we expect

$$w_{\mathbf{k}} = w(1/N). \tag{7.61}$$

From Eq. (7.59) we then obtain

$$\phi(w) = \tfrac{1}{2}(\tilde{\alpha}^{2}/\bar{\beta}), \tag{7.62}$$

where we use the abbreviation

$$\frac{1}{N^{2}}\sum_{\mathbf{k}\mathbf{k}'}\beta_{\mathbf{k}\mathbf{k}'} = \bar{\beta}.$$

We now compare the solution in which all modes participate, with the single mode solution for which

$$\tilde{\alpha}-\beta_{\mathbf{k}\mathbf{k}}w = 0 \tag{7.63}$$

holds, so that

$$\phi(w) = \tfrac{1}{2}(\tilde{\alpha}^{2}/\tilde{\beta}). \tag{7.64}$$

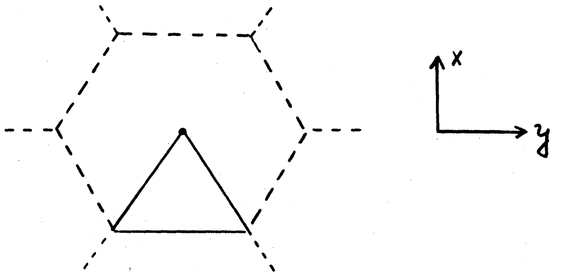

FIG. 9. Construction of hexagons from basic triangle (for details consult the text).

A comparison between Eqs. (7.62) and (7.64) reveals that the single mode has a greater probability than the multimode configuration. Our analysis can be generalized to different mode configurations leading again to the result that only a single mode is stable. This is in agreement with previous stability investigations by Schlüter *et al.* (1965) and others.

Let us discuss the form of the velocity field of such a single-mode configuration, using Eqs. (7.27) to (7.30). Choosing $\mathbf{k}$ in the x direction, we immediately recognize that the z component of the velocity field, u_z is independent of y, and has the form of a sine wave. Thus we obtain *rolls* as stable configurations. How do we explain the still more spectacular hexagons? To do this we include the cubic terms in (7.56) which stem from the spatial inhomogeneity in z direction. Admitting for the comparison only three modes with amplitudes A_i, A_i^{*}, $i = 1, 2, 3$, the potential function is given by

$$\Phi = \tilde{\alpha}(|\,A_1\,|^{2}+|\,A_2\,|^{2}+|\,A_3\,|^{2})-\delta(A_1{}^{*}A_2{}^{*}A_3{}^{*}+\text{c.c.})$$
$$-\tfrac{1}{2}\sum_{\mathbf{k}}k'\,\beta_{\mathbf{k}\mathbf{k}'}\,|\,A_{\mathbf{k}}\,|^{2}\,|\,A_{\mathbf{k}'}\,|^{2}, \tag{7.65}$$

where the $\mathbf{k}$ sums run over the triangle of Fig. 9 which arises from the condition $\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3 = 0$ and $|\,k_i\,| = \text{const.}$ [compare Eq. (7.33)].

To find the extremal values of Φ we take the derivatives of (7.65) with respect to A_i, A_i^{*}, and thus obtain six equations. Their solution is given by

$$A_i^{*} = A_i; \qquad A_1 = A_2 = A_3 = A. \tag{7.65a}$$

Using (7.65a) together with (7.27)–(7.35), we obtain e.g., $u_z(\mathbf{x})$. Concentrating our attention to its dependence on x, y, and using Fig. 9, we find (with $\mathbf{x}' = \pi/\sqrt{2}\mathbf{x}$)

$$u_z(\mathbf{x}) \propto A\{\exp(ix')+\exp(-ix')$$
$$+\exp i(-x'/2+y'\sqrt{3}/2)+\cdots, \tag{7.65b}$$

or in a more concise form

$$u_z(\mathbf{x}) \propto 2A\{\cos x'+\cos(\tfrac{1}{2}x'+\tfrac{1}{2}\sqrt{3}y')$$
$$+\cos(\tfrac{1}{2}x'-\tfrac{1}{2}\sqrt{3}y')\}. \tag{7.65c}$$

Using the solid line in Fig. 9 as an auxiliary pattern one easily convinces oneself that the hexagon of Fig. 9 is the elementary cell of $u_z(\mathbf{x})$ (7.65c).

In conclusion we discuss the probability of the occurrence of this hexagon compared with that of rolls. To this end we evaluate Eq. (7.65) with aid of (7.65a) which yields (using the explicit expression for A):

$$\phi_{\max}(A) = \hat{\beta}\{\tfrac{3}{2}\hat{\alpha}^2 + \tfrac{1}{2}\hat{\delta}^2\hat{\alpha} - A_{\max}(2\hat{\alpha}\hat{\delta} - \tfrac{1}{2}\hat{\delta}^3)\}. \tag{7.66}$$

Here we have used the abbreviations

$$\tfrac{1}{3}\hat{\beta} = \bar{\beta} \qquad \sum \beta_{k1} = \hat{\beta} \tag{7.67}$$

$$\hat{\alpha} = \tilde{\alpha}/\hat{\beta} \tag{7.68}$$

$$\hat{\delta} = \delta/\hat{\beta}. \tag{7.69}$$

We now discuss Eq. (7.66) for two different limiting cases:

$$(1) \qquad \hat{\delta}^2 \gg \hat{\alpha}. \tag{7.70}$$

In this case we obtain

$$\phi_{\max}(A) \approx \tfrac{1}{2}\hat{\beta}\hat{\delta}^3 A_{\max}. \tag{7.71}$$

$$(2) \qquad \hat{\delta}^2 \ll \hat{\alpha}. \tag{7.72}$$

In this case we obtain

$$\phi_{\max}(A) = \tilde{\alpha}^2/2\bar{\beta}. \tag{7.73}$$

A comparison between (7.71) or (7.73), respectively, with a single mode potential (7.62) reveals the following: for Rayleigh numbers $R > R_c$, which exceed R_c by a small amount, the hexagon configuration has a higher probability than the roll configuration. But a further increase of the Rayleigh number finally renders the single mode configuration (rolls) more probable.

VIII. FOKKER PLANCK EQUATION TREATMENT OF INTERACTING SOCIAL GROUPS

Intuitively it is rather obvious that formation of public opinion, actions of social groups, etc. are of a cooperative nature. On the one hand it appears extremely difficult if not completely impossible to put the treatment of such phenomena on a rigorous basis because the actions of individuals are determined by a number of (very often) unknown causes. Within the spirit of this article, we have seen that in systems with many subsystems there exist at least two levels of description: one which analyzes the individual system and its interaction with its surroundings, and another which describes the system's statistical behavior by using macroscopic variables. It is on this level that a quantitative description of interacting social groups becomes possible. This remark is, of course, basic to the whole field of insurance business, marketing, and economics, and is indeed mentioned in every introductory textbook on these subjects. In this chapter we will present a detailed mathematical model which has been used more recently by Weidlich (1971, 1972, 1973) to treat interacting social groups.

As a first step we have to seek the macroscopic variables describing a society. First of all we must look for the relevant characteristic features of an opinion. Of course "the opinion" is a very diffuse concept. However, similar to the measuring process in physics one can make a measurement of public opinion—e.g., by votes. In order to be as clear as possible we want to treat the simplest case where there are two kinds of opinions denoted by plus and minus. An obvious order parameter is the number of individuals n_+, n_- with the corresponding opinions $+$ and $-$, respectively. The basic concept now to be introduced is that the formation of the opinion, i.e., the change of the numbers n_+, n_- is a cooperative effect: The formation of the opinion of an individual is influenced by the presence of groups of people with the same or the opposite opinion. We thus assume that there exists a probability per unit time, for the change of the opinion of an individual from plus to minus or vice versa. We denote these transition probabilities by

$$p_{+-}(n_+, n_-) \qquad \text{and} \qquad p_{-+}(n_+, n_-). \tag{8.1}$$

We are interested in the probability distribution function $f(n_+, n_-, t)$. One may easily derive the following stochastic equation:

$$\begin{aligned}\frac{\partial f[n_+, n_-; t]}{\partial t} &\\ = -\{n_+p_{+-}[n_+, n_-] &+ n_-p_{-+}[n_+, n_-]\} f[n_+, n_-; t]\\ &+ (n_+ + 1)p_{+-}[n_+ + 1, n_- - 1]f[n_+ + 1, n_- - 1; t]\\ &+ (n_- + 1)p_{-+}[n_+ - 1, n_- + 1]f[n_+ - 1, n_- + 1; t].\end{aligned} \tag{8.2}$$

The crux of the present problem is, of course, not so much the solution of this equation, which can be done by standard methods, as the determination of the transition probability. As in problems in physics where not too much is known about the individual interaction, one may now introduce plausibility arguments to derive p. One possibility which has been discussed in detail by Weidlich is the following:

Assume that the rate of change of the opinion of an individual is enhanced by the group of individuals with the opposite opinion, and diminished by people of his own opinion. Assume furthermore that there is some sort of social over-all climate which either facilitates the change of opinion or else makes it more difficult. Finally one can think of external influences on each individual, e.g., information from abroad. For a physicist it is not too difficult to cast these assumptions into a mathematical form, if he thinks of the well known Ising model of the ferromagnet. Identifying the spin direction with the opinion $+$, $-$, we are led in analogy to the Ising model to put

$$\begin{aligned}p_{+-}[n_+, n_-] \equiv p_{+-}(q) &= \nu \exp\left\{\frac{-(Iq + H)}{\Theta}\right\},\\ &= \nu \exp\{-(kq + h)\},\\ p_{-+}[n_+, n_-] \equiv p_{-+}(q) &= \nu \exp\left\{\frac{+(Iq + H)}{\Theta}\right\},\\ &= \nu \exp\{+(kq + h)\},\end{aligned} \tag{8.3}$$

where I is a measure of the strengths of adaptation to neighbors. H is a preference parameter ($H > 0$ means that opinion + is preferred to −), Θ is a collective climate parameter corresponding to k_BT in physics (k_B is the Boltzmann constant and T the temperature), ν is the frequency of the "flipping" processes. Finally

$$q=(n_+-n_-)/2n, \qquad n=n_++n_-. \tag{8.4}$$

For a quantitative treatment of Eq. (8.2) we assume social groups big enough so that q may be treated as a continuous parameter. Transforming (8.2) to this continuous variable and putting

$$\begin{aligned} w_{+-}(q) &\equiv n_+p_{+-}[n_+,n_-]=n(\tfrac{1}{2}+q)p_{+-}(q), \\ w_{-+}(q) &\equiv n_-p_{-+}[n_+,n_-]=n(\tfrac{1}{2}-q)p_{-+}(q), \end{aligned} \tag{8.5}$$

we transform (8.2) into a partial differential equation (see e.g., Sec. V of this review article). Its solution may be found by quadratures in the form

$$f_{st}(q)=cK_2^{-1}(q)\exp\left\{2\int_{-1/2}^{q}\frac{K_1(y)}{K_2(y)}\,dy\right\} \tag{8.6}$$

with

$$\begin{aligned} K_1(q) &= \nu\{\sinh(kq+h)-2q\cosh(kq+h)\} \\ K_2(q) &= (\nu/n)\{\cosh(kq+h)-2q\sinh(kq+h)\}. \end{aligned} \tag{8.7}$$

As one may expect from a direct knowledge of the Ising model, there are typically two results. One result corresponds to the high temperature limit: on account of rather frequent changes of opinion we find a centered distribution of opinions. If the social climate factor Θ is lowered or if the coupling strengths between individuals is increased, two pronounced groups of opinions occur which clearly describe the by now well known "polarization phenomenon" of society. It should be noted that the present model allows us to explain, at least in a qualitative manner, further processes, e.g., unstable situations where the social climate parameter is changed to a critical value. Here suddenly large groups adhering to an opinion are formed which are dissolved only slowly, and it remains uncertain which group (+ or −) finally wins. Using the considerations of Sec. II it is obvious that again here concepts of phase-transition theory become important, like critical slowing down (remember the duration of the 1968 French student revolution, which led Weidlich and the present author to a discussion about the possibility of such analogies), critical fluctuations, etc. As has been stressed by Weidlich, such statistical descriptions certainly do not allow unique predictions due to the stochastic nature of the process described. Nevertheless such models are most valuable in understanding general features of cooperative behavior even of human beings, though the behavior of a single individual may be extremely complicated and not accessible to a mathematical description.

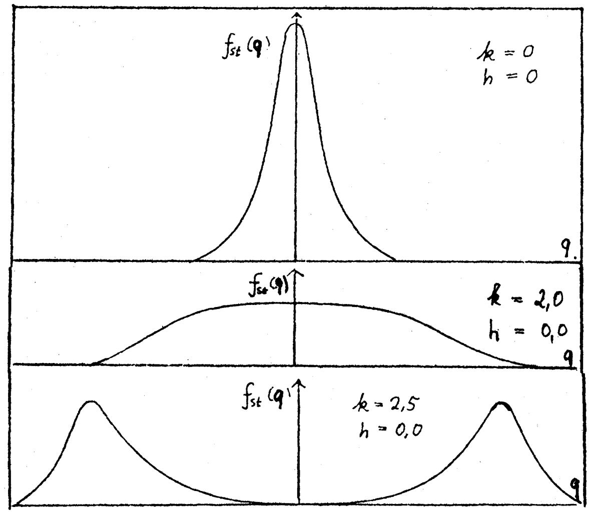

FIG. 10. (a) Centered distribution in the case of rather frequent changes of opinion (independent decision). (b) Distribution at the transition between independent and strongly adaptive decision. (c) "Polarization phenomenon" in the case of strong neighbor-neighbor interaction.

The model described above has been generalized by Weidlich to several interesting examples, for instance interaction of a small group with a big group (e.g., management and employees, or government and population etc.). Such treatments reveal in particular how, and how quickly, public opinion may change. It is quite obvious that many generalizations can be now worked out, some of which are already given by further papers of Weidlich (1972, 1973).

IX. NEURON NETWORKS

In the present chapter we want to demonstrate how the concept of macroscopic variables or order parameters proves to be useful in a description of cooperative phenomena in neuron networks. We follow closely the work by Wilson and Cowan (1972) and Wilson (1973) on a homogeneous cortical tissue model. We leave aside those papers which deal with the neurons itself though they are also very appealing to physicists [see e.g. Güttinger (1972, 1973), Hahn and Güttinger (1972)]. One may readily convince oneself that neuron activity in the cerebral cortex must be cooperative in nature. This follows from the fact that nerve cells can become active only if they receive signals from at least 10 other cells, in a finite time interval (of the order of 10 msec). This property evidently suppresses random noise and gives rise to cooperative effects. One may further show that there is a local redundancy of cell function which allows us to treat the functioning of the cortical tissue as a two-dimensional problem.

Actual calculations have been performed with respect to a one-dimensional model in the framework of a deterministic dynamical system which neglects the impact of noise.[24] The model starts from the fact that there exist two types of cells, namely excitatory and inhibitory cells. Their distribution over the tissue is taken to be homogeneous with surface densities ρ_e and ρ_i, respectively. We denote by $E(x,t)$ the excitatory neuron activity, or more precisely $\rho_eE\,dx\,dt$ is

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[24] Here we have in mind the conventional concept of "noise." Landauer (private communication) has defined a generalized "noise" in the following sense. "Noise" may be anything which causes ensemble members which are together initially to depart from each other with time. In this sense the distribution function $D_e(\theta)$ [compare Eq. (9.3)], just like a lack of reproducibility in computer components, is really noise. It causes δ-function distributions to become spread out, just as thermal agitation does.

the number of excitatory cells becoming active during the time interval dt in the space interval dx, or in short, E is the transition rate of the neuron to its active state. In a similar way we define the inhibitory neuron activity $I(x, t)$. In the following we will derive equations for E and I using plausability arguments.

Consider a single cell (or a distribution of equivalent cells). It is known that the so-called post-synaptic potential PSP generated in that cell is caused by activity in all other cells. On the other hand the post-synaptic potential, after reaching a certain threshold, allows the cell to emit signals. We denote the transfer functions transferring signals between excitatory and inhibitory cells by $\beta_{e,e}$, $\beta_{e,i}$, $\beta_{i,e}$, $\beta_{i,i}$, and assume that postsynaptic effects are additive. For the corresponding processes the postsynaptic potential of excitatory cells reads

$$PSP_e(x,t) = \int_{-\infty}^{\infty} \beta_{ee}(|x-x'|)E(x',t)\,dx' - \int_{-\infty}^{\infty} \beta_{ie}(|x-x'|)I(x',t)\,dx' + P(x,t) \tag{9.1}$$

where $P(x, t)$ is an external input for the tissue from other parts of the brain or from sense organs. Denoting spatial convolution by $\otimes$, Formula (9.1) may be written as

$$PSP_e(x,t) = \beta_{ee}\otimes E - \beta_{ie}\otimes I + P(x,t). \tag{9.2}$$

Equation (9.1) assumes that the transmission of signals occurs instantaneously.

We now derive the equation for E. As already mentioned a cell becomes active only if its PSP exceeds a threshold value, Θ, and furthermore if it is sensitive, i.e., if it is not refractory. The number of cells becoming active is proportional to the proportion of excited cells above threshold times the number which is sensitive. If there is a distribution of threshold $D_e(\Theta)$ the number of cells S_e receiving superthreshold excitation is given by

$$S_e(PSP_e) = \int_0^{PSP_e} D_e(\Theta)\,d\Theta. \tag{9.3}$$

A typical function (9.3) is plotted in Fig. 11. Apparently it describes some sort of saturation behavior. The proportion of excitatory cells at x which are sensitive at the time $t+\delta t$ is given by $1 - rE(x,t)$, where r is the duration of the refractory period. We are now in a position to establish the equation for E. If there were no signals from other cells, E would decay within a time τ so that its equation would read

$$\tau(dE/dt) = -E. \tag{9.4}$$

On the other hand, the rate at which cells become active is given by $(1-rE)S(PSP_e)$. Replacing PSP_e by Eq. (9.1) we obtain the final equation

$$\tau(\partial E/\partial t) = -E + (1-rE)S[\beta_{ee}\otimes E - \beta_{ie}\otimes I + P(x,t)]. \tag{9.5}$$

In a similar manner, one obtains for the inhibitory activity, the equation

$$\tau(\partial I/\partial t) = -I + (1-rI)S[\beta_{ei}\otimes E - \beta_{ii}\otimes I - Q(x,t)]. \tag{9.6}$$

Equations (9.5) and (9.6) are nonlinear equations for E and I. They have forms which also occur in physical problems and must be solved by computer. Wilson and Cowan have used the following explicit forms for S and β.

$$S(\mathrm{PSP}) = \{1+\exp[-a(PSP-\Theta)]\}^{-1}, \tag{9.7}$$

$$\beta(|x-x'|) = b\exp(-|x-x'|/\sigma). \tag{9.8}$$

Equations of that sort are typical for active circuits.

Three different kinds of modes were found by computer solutions.

(1) Stable and spatially inhomogeneous steady states. Such states may play a role in active short term memory,

(2) Limit cycle type oscillations in response to maintained stimulation. For sufficiently broad stimuli one can obtain edge enhancement. This class of solutions includes coherent oscillation and frequency demultiplication (compare Fig. 12).

(3) An active transient mode which remains spatially localized. We mention that through this model comprising 1), 2), 3) a number of experiments on vision for instance but also on other effects, find their explanation. It would take us beyond the goal of the present article to enter into

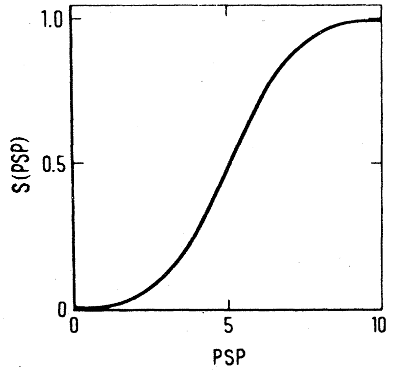

FIG. 11. Plot of a typical sigmoidal function. The particular function shown here is the logistic curve: $S(PSP) = 1/[1+\exp(-a(PSP-\theta))]$ with $\theta = 5$, $a = 1$. (After H. R. Wilson (1973) in *Synergetics*.)

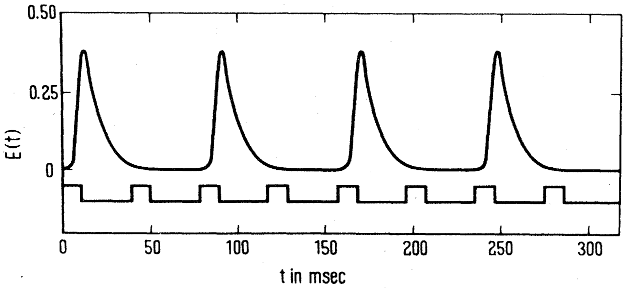

FIG. 12. Frequency demultiplication in the neural response to a stimulus pulse train. Each stimulus pulse had a narrow, rectangular spatial profile. (After H. R. Wilson (1973) in *Synergetics*.)

the details of these interpretations. It seems important to note in our present context, however, that reasonable modelling may explain a number of observed brain responses.

PART II: THE MATHEMATICAL APPARATUS

While in the first part we have given a number of explicit examples of cooperative effects in systems far from thermal equilibrium, in part II we want to present a coherent account of the methods enabling us to deal with such systems. We have tried to include in particular very recent developments, such as methods for solving master equations and Fokker–Planck equations. This second part is organized as follows: Sections X–XII deals with classical systems; Secs. XIII–XV with quantum systems. In Sec. XVI we present the method of quantum classical correspondence which allows us to transform the quantum mechanical problem into a c-number problem. For the article to be self-contained we start with a few reminders of concepts of probability theory.

X. SOME BASIC CONCEPTS OF PROBABILITY THEORY WITH APPLICATIONS TO PHYSICS AND RELATED DICIPLINES[25]

A. Random variables and probability densities. Definitions

Consider a *random variable* ξ which may adopt continuous values. Each measurement gives rise to a realization of the random variable. Those realizations are denoted by $\xi_1, \xi_2, \cdots$ We define the *mean value* (expectation value) by

$$\langle\xi\rangle = \lim_{n\to\infty} \frac{\xi_1 + \xi_2 + \cdots \xi_n}{n} \tag{10.1}$$

and that of an arbitrary function g of ξ by

$$\langle g(\xi)\rangle = \lim_{n\to\infty} (1/n) \sum_{\nu=1}^{n} g(\xi_\nu). \tag{10.2}$$

Using Dirac's δ function we define the *probability density* by

$$f_\xi(q) = \langle \delta(\xi - q)\rangle. \tag{10.3}$$

Because often the value of q is denoted by the same letter as the random variable ξ itself, we replace $f_\xi(q)$ by $f_\xi(\xi)$. Dropping the redundant subscript we obtain $f(\xi)$. The probability density must be normalized

$$\int f(\xi)\, d\xi = 1. \tag{10.4}$$

The *mean value* (expectation value) of a function $g(\xi)$ is obtained by means of f through the formula

$$\langle g(\xi)\rangle = \int g(\xi) f(\xi)\, d\xi. \tag{10.5}$$

The *characteristic function* is defined by

$$\Theta_\xi(u) = \langle \exp(iu\xi)\rangle = \int \exp(iu\xi) f(\xi)\, d\xi. \tag{10.6}$$

Moments are defined by

$$m_n = \langle \xi^n\rangle; \qquad n = 1, 2, \cdots. \tag{10.7}$$

They may be obtained from the characteristic functions as derivatives

$$m_n = (1/i^n)[d^n\Theta_\xi(u)/du^n]\,|_{u=0}. \tag{10.8}$$

Cumulants k_n are defined by

$$\Theta_\xi(u) = \exp\left\{\sum_{n=1}^{\infty} \frac{(iu)^n}{n!} k_n\right\}. \tag{10.9}$$

Taking the logarithm of (10.9) on both sides, the coefficients k_n of the Taylor expansion with respect to u are given by

$$k_n = (1/i^n)[d^n \ln\Theta_\xi(u)/du^n]\,|_{u=0}. \tag{10.10}$$

The first cumulants read

$$k_1 = m_1, \tag{10.11}$$

$$k_2 = m_2 - m_1^2. \tag{10.12}$$

If ξ has *discrete realizations* μ, one has to replace the δ function $\delta(\xi - q)$ by $\delta_{\xi,\mu}$, and correspondingly define the average value of $g(\xi)$ by

$$\langle g(\xi)\rangle = \sum_\mu g(\mu) f(\mu). \tag{10.13}$$

If ξ has both continuous and discrete values one has to replace the integrals by Stieltjes' integrals. The above definitions are readily generalized to several random variables $\xi_1, \cdots, \xi_r$. (Note the change of definition of the ξ's, because the indices now denote no more realization of the single stochastic random variable but distinguish different random variables!).

The *probability density* is defined by

$$f_{\xi_1\cdots\xi_r}(q_1\cdots q_r) = \langle \delta(\xi_1 - q_1)\cdots\delta(\xi_r - q_r)\rangle \tag{10.14}$$

and the *average* of an arbitrary function g of ξ_1 to ξ_r by

$$\langle g(\xi_1,\cdots\xi_r)\rangle = \int\cdots\int f(\xi_1,\cdots\xi_r) g(\xi_1,\cdots\xi_r)\, d\xi_1\cdots d\xi_r. \tag{10.15}$$

Equation (10.14) implies the *normalization condition*

$$\int\cdots\int f(\xi_1,\cdots,\xi_r)\, d\xi_1\cdots d\xi_r = 1. \tag{10.16}$$

We introduce the abbreviation

$$f(\xi_1) = \int f(\xi_1, \xi_2)\, d\xi_2, \tag{10.17}$$

where $f(\xi_1)$ gives the probability of finding ξ_1 irrespective which value of ξ_2 is accepted. We then define the *conditional probability density* as follows: for two variables we have

$$f(\xi_1 \mid \xi_2) = f(\xi_1, \xi_2)/f(\xi_2) \tag{10.18}$$

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[25] Readers interested in more details are referred to the excellent review articles and books by Lax (1960, 1966a, b) and Stratonovich (1963, 1967), respectively.

and in the general case we define the *conditional probability density*

$$f(\xi_1,\cdots,\xi_k \mid \xi_{k+1},\cdots,\xi_r) = f(\xi_1,\cdots,\xi_r)/f(\xi_{k+1},\cdots,\xi_r), \tag{10.19}$$

where

$$f(\xi_{k+1},\cdots,\xi_r) = \int\cdots\int f(\xi_1,\cdots,\xi_r)\, d\xi_1\cdots d\xi_k. \tag{10.20}$$

If we let the indices $1,\cdots,r$ become continuous variables and identify them with the time t, the set of random variables ξ may be described as a random function $\xi(t)$. Now taking a discrete time sequence $t_1,\cdots,t_r$, we may transcribe the definition (10.14) into the definition of the probability density of a random function

$$f_r(q_1,\cdots,q_r;t_1,\cdots,t_r) = \langle \delta(q_1-\xi(t_1))\cdots\delta(q_r-\xi(t_r))\rangle \tag{10.21}$$

Correspondingly the characteristic function is defined by

$$\Theta_r(u_1,\cdots,u_r;t_1,\cdots,t_r) = \langle \exp i(u_1\xi(t_1)+\cdots+u_r\xi(t_r))\rangle, \tag{10.22}$$

and the cumulants by

$$\Theta_r(u_1,\cdots,u_r;t_1,\cdots,t_r) = \exp\left\{\sum_{s=1}^{\infty}\frac{i^s}{s!}\sum_{\alpha_1,\cdots\alpha_s=1}^{r} k_s(t_{\alpha_1},\cdots,t_{\alpha_s})u_{\alpha_1}\cdots u_{\alpha_s}\right\} \tag{10.23}$$

in straightforward generalization of the corresponding definitions (10.6) and (10.9), respectively. We now come to a very important notation. The random function $\xi(t)$ is said to represent a *Gaussian process* if all cumulants other than the first two vanish, i.e., if

$$k_3 = k_4 = \cdots = 0 \tag{10.24}$$

holds. In that case the characteristic function is represented by

$$\Theta_r(u_1,\cdots,u_r;t_1,\cdots,t_r) = \exp\{i\sum_{\alpha=1}^{r} k_1(t_\alpha)u_\alpha - \tfrac{1}{2}\sum_{\alpha,\beta=1}^{r} k_2(t_\alpha,t_\beta)u_\alpha u_\beta\}. \tag{10.25}$$

If one defines moments in generalization of Eq. (10.8) one extablishes immediately from Eq. (10.25) that all moments may be expressed by the first two cumulants 1, 2 or, because the first cumulants may be expressed by the first and second moments, all higher moments may be expressed by the first two moments. If $\xi_1,\cdots,\xi_r$ have discrete realizations one has to replace the integrals by sums, and if both discrete and continuous realizations are present one has to replace the integrals by Stieltjes integrals.

B. Markov process and stochastic equations

We now come to a second definition which plays an important role in many practical applications. We therefore begin with a motivation for this analysis. As we have seen, in practical examples we are often dealing with macroscopic variables or order parameters which change slowly compared to the motion of their subsystems. Or using the still more familiar example of a Brownian particle, the velocity at each moment of the Brownian particle depends on the last push it has received. We now define this property in mathematical terms and call it *Markov process*. Let $q(t)$ be a random process and $(t_1, t_2\cdots t_n)$ be a given time sequence with

$$t_1 > t_2 \cdots > t_n \tag{10.26}$$

We consider the conditional probability density

$$f[q(t_1) \mid q(t_2),\cdots,q(t_n)] = \frac{f_n[q(t_1),\cdots,q(t_n)]}{f_{n-1}[q(t_2),\cdots,q(t_n)]}. \tag{10.27}$$

A process is called Markovian if the left-hand side of Eq. (10.27) depends only on $q(t_2)$ and not on the preceding process. Thus we may write instead of (10.27) [with $q_i \equiv q(t_i)$]

$$f(q_1 \mid q_2,\cdots,q_n) = p_{t_1t_2}(q_1,q_2) \qquad (n\geq 2). \tag{10.28}$$

We call

$$p_{t_1t_2}(q_1,q_2) = w(q_1 \mid q_2), \qquad t_1 > t_2 \tag{10.29}$$

the *transition probability*. Multiplying Eq. (10.27) on both sides by f_{n-1} and then applying this formula recurrently using (10.29) we find the formula

$$f(q_1,\cdots,q_n) = p_{t_1t_2}(q_1,q_2)p_{t_2t_3}(q_2,q_3)\cdots p_{t_{n-1}t_n}(q_{n-1},q_n)\, f(q_n). \tag{10.30}$$

Using the definitions (10.19), (10.20) and (10.29) one immediately obtains the *Chapman–Kolmogorov equation*

$$\int p_{t_1t_2}(q_1,q_2)p_{t_2t_3}(q_2,q_3)\, dq_2 = p_{t_1t_3}(q_1,q_3); \qquad (t_1>t_2>t_3). \tag{10.31}$$

It may be generalized to an n-dimensional vector $\mathbf{q}$ and then reads

$$\int\cdots\int p_{t_1t_2}(\mathbf{q}_1,\mathbf{q}_2)p_{t_2t_3}(\mathbf{q}_2,\mathbf{q}_3)\, d^nq_2 = p_{t_1t_3}(\mathbf{q}_1,\mathbf{q}_3); \qquad (t_1>t_2>t_3). \tag{10.32}$$

If q acquires only discrete values the integrals must be replaced by sums. Multiplying both sides of Eq. (10.31) by $f(q_3)$ and integrating we find another form of the Chapman–Kolmogorov equation, namely

$$f(q,t) = \int p_{t,t_0}(q,q_0)\, f(q_0,t_0)\, dq_0 \tag{10.33}$$

in one dimension, or

$$f(\mathbf{q},t) = \int\cdots\int p_{t;t_0}(\mathbf{q},\mathbf{q}_0)\, f(\mathbf{q}_0,\mathbf{t}_0)\, d^nq_0 \tag{10.34}$$

in n-dimensions, or if discrete values are present

$$f(n_1,\cdots,n_r,t)$$
$$\sum_{m_1,\cdots,m_r} p_{t,t_0}(n_1,\cdots,n_r;m_1,\cdots,m_r)\,f(m_1,\cdots,m_r,t_0). \tag{10.35}$$

We obtain the so-called stochastic equation if we take on both sides of (10.35) the time derivative ($t = t_0 + \tau$ with $\tau \rightarrow 0$).

$$\begin{aligned}\dot f(n_1,\cdots,n_r;t) &= \sum_{m_1,\cdots,m_r} \dot p_{t,t_0}(n_1,\cdots,n_r;m_1,\cdots,m_r)\,|_{t=t_0}\\ &\quad\times f(m_1,\cdots,m_r;t).\end{aligned} \tag{10.36}$$

Denoting the transition probability per unit time by W we find

$$\begin{aligned}\dot f(n_1,\cdots,n_r;t) &= \sum_{m_1,\cdots,m_r} W(n_1,\cdots,n_r;m_1,\cdots,m_r)\,f(m_1,\cdots,m_r;t).\end{aligned} \tag{10.37}$$

We now return to the case in which q is a continuous variable. Then one may deduce from Eq. (10.33) by a formal expansion in $(q - q_0)$ (compare also Sec. XI.A) the *stochastic (kinetic) equation*

$$\dot f(q) = \sum_{s=1}^{\infty} \frac{1}{s!}\left(-\frac{\partial}{\partial q}\right)^s [K_s(q)\,f(q)] \tag{10.38}$$

with the definitions

$$K_s(q) = \lim_{\tau\to 0}\,[m_s(q)/\tau] \tag{10.39}$$

and

$$m_s(q) = \langle (q_\tau - q)^s \rangle. \tag{10.40}$$

The formulas (10.38)–(10.40) may be used rather simply e.g., to derive the Fokker—Planck equation from Langevin equations by determining q_τ for small values from these latter equations. The derivation of Eq. (10.38) from (10.33) may be justified in several explicit cases on physical grounds. For instance one introduces the inverse volume as expansion parameter (compare Sec. XI). It should be noted, however, hat such an expansion may require an infinite number of derivatives, for instance near instabilities (phase transitions). On the other hand in many important cases it is sufficient to terminate the expansion (10.38) after the first two derivatives. If $K_3, K_4, \cdots = 0$, the process is called a *continuous Markov process* and one obtains the *Fokker–Planck equation*

$$\dot f(q) = -(\partial/\partial q)[K_1(q)\,f(q)] + \tfrac{1}{2}(\partial^2/\partial q^2)[K_2(q)\,f(q)]. \tag{10.41}$$

If the initial distribution function at $t = t_0$ is a δ function

$$f_{t_0}(q) = \delta(q - q_0), \tag{10.42}$$

we put

$$f(q) = p_{t,t_0}(q, q_0), \tag{10.43}$$

and find the so-called "forward Kolmogorov equation"

$$\begin{aligned}\frac{\partial p_{t,t_0}(q,q_0)}{\partial t} &= -\frac{\partial}{\partial q}[K_1(q)\,p_{tt_0}(q,q_0)]\\ &\quad+\frac{1}{2}\frac{\partial^2}{\partial q^2}[K_2(q)\,p_{tt_0}(q,q_0)]\end{aligned} \tag{10.44}$$

subject to the initial condition

$$p_{t_0t_0}(q, q_0) = \delta(q - q_0). \tag{10.45}$$

The "backward Kolmogorov equation" is defined as the equation adjoint to the Fokker–Planck equation

$$\begin{aligned}\frac{\partial p_{tt_0}(q,q_0)}{\partial t_0} &= -\frac{\partial p_{tt_0}(q,q_0)}{\partial q_0}K_1(q_0)\\ &\quad-\frac{1}{2}\frac{\partial^2 p_{tt_0}(q,q_0)}{\partial q_0^2}K_2(q_0).\end{aligned} \tag{10.46}$$

The preceding considerations may be generalized to many variables $q_1, \cdots, q_m$. The multidimensional stochastic equation reads

$$\begin{aligned}\dot f(q_1,\cdots,q_m) &= \sum_{\nu_1=1}^{\infty}\sum_{\nu_2=1}^{\infty}\cdots\sum_{\nu_m=1}^{\infty}(-1)^{\nu_1+\nu_2+\cdots+\nu_m}\frac{1}{(\nu_1!\nu_2!\cdots\nu_m!)}\\ &\quad\times\left(\frac{\partial}{\partial q_1}\right)^{\nu_1}\cdots\left(\frac{\partial}{\partial q_m}\right)^{\nu_m}[K^{\nu_1,\cdots,\nu_m}(q_1,\cdots,q_m)\,f(q_1,\cdots,q_m)]\end{aligned} \tag{10.47}$$

with

$$\begin{aligned}K^{\nu_1,\cdots,\nu_m}(q_1,\cdots,q_m) &= \lim_{\tau\to 0}(1/\tau)\langle (q_{1\tau}-q_1)^{\nu_1}\cdots(q_{m\tau}-q_m)^{\nu_m}\rangle.\end{aligned} \tag{10.48}$$

When only the first two derivatives are kept, Eq. (10.47) reduces to the *Fokker–Planck equation*

$$\begin{aligned}\dot f(q_1,\cdots,q_m) &= -\sum_{\alpha=1}^{m}\frac{\partial}{\partial q_\alpha}[K_\alpha(q_1,\cdots,q_m)\,f(q_1,\cdots,q_m)]\\ &\quad+\tfrac{1}{2}\sum_{\alpha,\beta=1}^{m}\frac{\partial^2}{\partial q_\alpha\,\partial q_\beta}[K_{\alpha\beta}(q_1,\cdots,q_m)\,f(q_1,\cdots,q_m)],\end{aligned} \tag{10.49}$$

where the *drift coefficients* are given by

$$K_\alpha(q_1,\cdots,q_m) = \lim_{\tau\to 0}(1/\tau)\langle (q_{\alpha\tau} - q_\alpha)\rangle, \tag{10.50}$$

and the *diffusion coefficients* by

$$K_{\alpha\beta}(q_1,\cdots,q_m) = \lim_{\tau\to 0}(1/\tau)\langle (q_{\alpha\tau}-q_\alpha)(q_{\beta\tau}-q_\beta)\rangle. \tag{10.51}$$

XI. SOLUTIONS OF STOCHASTIC EQUATIONS

A. Reduction of the Chapman-Kolmogorov equation to a Fokker–Planck equation with "normal fluctuations"

1. One-dimensional example

First we indicate by means of an one-dimensional example how the Fokker–Planck equation (10.41) may be derived by an expansion of the so-called master equation in a power series of $\epsilon = 1/V$, where V is the volume of the system. Taking the time derivative of the Chapman–Kolmogorov equation (10.33) we obtain, in a way which is completely analogous to the method leading to (10.37), for discrete values:

$$\dot{f}(q;t) = \int W(q, q_0; t)\, f(q_0; t)\, dq_0, \tag{11.1}$$

where

$$W(q, q_0; t) = (d/dt) p_{t,t_0}(q, q_0)\,|_{t=t_0}. \tag{11.2}$$

We cast Eq. (11.1) into the usual form of the master equation by putting

$$W(q, q_0; t) = w(q, q_0; t) - \delta(q - q_0) \int w(q', q; t)\, dq'. \tag{11.3}$$

Equation (11.1) then reads

$$\dot{f}(q, t) = \int w(q, q_0, t)\, f(q_0, t)\, dq_0 - f(q, t) \int w(q', q, t)\, dq'. \tag{11.4}$$

We write the transition probability $w(q', q; t)$ in the form

$$\hat{w}(q, r, t); \qquad q' = q + r. \tag{11.5}$$

We now assume that the probability of such a transition taking place in an infinitely short time interval is proportional to the size V and is determined by the intensive coordinate $\eta = q/V$ so that we write

$$\hat{w}(q, r, t) = V\tilde{w}(\eta, r, t). \tag{11.6}$$

Thus Eq. (11.4) is transformed into

$$\epsilon(\partial/\partial t)\, f(\eta, t) = -\int \tilde{w}(\eta, r, t)\, dr f(\eta, t) + \tilde{w}(\eta - \epsilon r, r, t)\, dr f(\eta - \epsilon r, t). \tag{11.7}$$

(Incidentally we make the replacement $f(q, t) \rightarrow Vf(\eta, t)$). Expanding the right-hand side of Eq. (11.7) into a series of powers of ϵ we find

$$\frac{\partial}{\partial t} f(\eta, t) = \sum_{n=1}^{\infty} \frac{(-)^n}{n!} \epsilon^{n-1} \left(\frac{\partial}{\partial \eta}\right)^n c_n(\eta, t)\, f(\eta, t), \tag{11.8}$$

with

$$c_n(\eta, t) = \int r^n \tilde{w}(\eta, r, t)\, dr. \tag{11.9}$$

Equation (11.8) is also called the Kramers–Moyal expansion. The extension to many variables is straightforward.

Following van Kampen (1961) and Kubo *et al.* (1973) we put

$$\eta = y(t) + \epsilon^{1/2}\xi, \tag{11.10}$$

where ξ is assumed to be of order V^0. Here $y(t)$ is chosen to satisfy the equation

$$\dot{y}(t) = c_1(y), \tag{11.11}$$

where c_1 is defined in Eq. (11.9). Putting further $f(\eta, t) = \bar{f}(\xi, t)$, Eq. (11.8) is transformed into

$$\frac{\partial}{\partial t} \bar{f}(\xi, t) = -\epsilon^{-1/2} \frac{\partial}{\partial \xi} [c_1(y + \epsilon^{1/2}\xi) - c_1(y)] \bar{f}(\xi, t) + \sum_{n=2}^{\infty} (-)^n \frac{\epsilon^{(n-2)/2}}{n!} \left(\frac{\partial}{\partial \xi}\right)^n c_n(y + \epsilon^{1/2}\xi)\, \bar{f}(\xi, t) \tag{11.12}$$

which in the limit $\epsilon \rightarrow 0$ reduces to

$$(\partial/\partial t)\, \bar{f}(\xi, t) = -(\partial/\partial \xi) c_1'(y) \xi \bar{f} + \tfrac{1}{2}(\partial^2/\partial \xi^2) c_2(y) \bar{f}$$
$$c_1' = dc_1(y)/dy \tag{11.13}$$

which has as solution a Gaussian distribution

$$\bar{f} = N \exp\{-(1/2\epsilon)\sigma^{-1}[\eta - y(t)]^2\} \tag{11.14}$$

(N: normalization constant) with $y(t)$ and $\sigma(t)$ determined by Eqs. (11.11) and

$$\dot{\sigma}(t) = 2c_1'(y)\sigma(t) + c_2(y), \tag{11.15}$$

respectively.

2. The general case

The above procedure can be readily generalized to many variables [van Kampen (1961; Kubo *et al.* (1973)]: The distribution function $f(\eta, t)$ which fulfills the master equation (10.37) with continuous variables can be written [in the same ($\epsilon \rightarrow 0$) approximation as in XI.A.1] as

$$f(\eta, t) = N \exp\{-(1/2\epsilon) \sum (\sigma^{-1})_{jk} [\eta_j - y_j(t)] \times [\eta_k - y_k(t)] + \cdots\}, \tag{11.16}$$

where N is the (in general time-dependent) normalization constant, and the coefficients σ_{jk} and y_j obey the equations

$$\dot{y}_j(t) = c_{1j}(y), \tag{11.17}$$

with

$$c_{1j}(y) = \int dr r_j \tilde{w}(y_1, \cdots, y_n, r_1, \cdots, r_n), \tag{11.18}$$

and

$$\dot{\sigma}_{jk}(t) = \sum_l \left(\sigma_{jl} \frac{\partial c_{1k}}{\partial y_l} + \frac{\partial c_{1j}}{\partial y_l} \sigma_{lk}\right) + c_{2jk}, \tag{11.19}$$

with

$$c_{2jk}(y) = \int dr r_j r_k w(y_1, \cdots, y_n, r_1, \cdots, r_n), \tag{11.20}$$

respectively, [compare also Eq. (10.51)].

The question of whether Eq. (11.16) remains valid in the neighborhood of critical points seems to require further investigations. Furthermore, in other applications the expansion parameter ϵ may have a different meaning and the decomposition (11.6) may not be permissible. We mention a few examples: In the case of single and multimode lasers it was shown [Haken (1970a) p. 154, Haken and Vollmer (1971)] that one may use an ordinary Fokker–Planck equation, but with nonlinear drift coefficients. In certain electronic devices higher-order diffusion terms must be included if the drift coefficients are nonlinear [van Kampen (1961)]. Recently, the above procedure has been considerably generalized by Mori (to be published), to treat different classes of dynamic equations in which the "coherent" motion and the fluctuations scale in a more general way than described in the foregoing.

B. Time-dependent and time-independent solution of the Fokker–Planck equation, if the drift coefficients are linear in the coordinates and the diffusion coefficients constant

In a certain class of applications one may assume that drift coefficients can be linearized around certain stable values of the coordinates and that the diffusion coefficients are independent of the coordinates. If we denote the elongation from the equilibrium positions by q_j, the corresponding Fokker–Planck equation reads

$$\frac{\partial f}{\partial t}+\sum_{ij} c_{ij}\frac{\partial}{\partial q_i}(q_j f)=\tfrac{1}{2}\sum_{ij} Q_{ij}\frac{\partial^2 f}{\partial q_i\,\partial q_j}. \tag{11.21}$$

We abbreviate $q_1,\cdots,q_N$ by $\mathbf{q}$. The Green's function of (11.21) must fulfill the initial condition

$$G(\mathbf{q},\mathbf{q}',0)=\prod_j \delta(q_j-q_j'). \tag{11.22}$$

The solution of Eq. (11.21) with Eq. (11.22) reads explicitly (see e.g. Wang and Uhlenbeck (1945))

$$\begin{aligned}G(\mathbf{q},\mathbf{q}',t) &= (\pi^n Det\boldsymbol{\sigma}(t))^{-1/2}\\ &\times \exp\{-\sum_{ij}(\sigma^{-1})_{ij}(q_{ij}-\sum_k b_{ik}(t)q_k')\\ &\times (q_j-\sum_l b_{jl}(t)q_l')\},\end{aligned} \tag{11.23}$$

where

$$\boldsymbol{\sigma}=(\sigma_{ij}), \tag{11.24}$$

$$\sigma_{ij}(t)=\sum_{sr}[\delta_{is}\delta_{jr}-b_{is}(t)b_{jr}(t)]\sigma_{sr}(\infty). \tag{11.25}$$

The function b_{is} which occur in Eq. (11.25) obey the equations

$$\dot{b}_{is}=\sum_j C_{ij}b_{js}, \tag{11.26}$$

with the initial conditions

$$b_{js}(0)=\delta_{js}. \tag{11.27}$$

Here $\boldsymbol{\sigma}(\infty)$ is determined by

$$\mathbf{C}\boldsymbol{\sigma}(\infty)+\boldsymbol{\sigma}(\infty)\mathbf{C}^T=-2\mathbf{Q}, \tag{11.28}$$

where we have used the abbreviations

$$\mathbf{C}=(C_{ij}), \tag{11.29}$$

$$\mathbf{Q}=(Q_{ij}), \tag{11.30}$$

and the superscript T denotes the transposed matrix. In particular the stationary solution reads

$$\begin{aligned}f(q) &= G(q,q',\infty)=(\pi^n Det\boldsymbol{\sigma}(\infty))^{-1/2}\\ &\times \exp\{-\sum_{ij}(\sigma^{-1})_{ij}(\infty)q_iq_j\}\end{aligned} \tag{11.31}$$

C. Time-independent and time-dependent solution of the Fokker–Planck equation of a system weakly coupled to reservoirs

To elucidate our method (Haken 1973c), we first treat the following model:

1. Fokker–Planck equation of a system of interacting Brownian particles[26]

We consider N particles which interact with each other and which may also be subject to "coherent" external forces. Denoting the coordinate and moment of particle j by q_j, p_j, respectively, we describe their motion by a Hamiltonian $H(p_1,\cdots,p_N,q_1,\cdots q_N)$. Furthermore, we assume that these particles suffer collisions with other much lighter particles and that these collisions may be described as in the theory of Brownian motion by a friction force $-\gamma_j p_j$ and a fluctuation force F_j. The Langevin equations then read (compare Sec. XII)

$$\dot{p}_j=-(\partial H/\partial q_j)-\gamma_j p_j+F_j, \tag{11.32}$$

$$\dot{q}_j=(\partial H/\partial p_j). \tag{11.33}$$

The Fokker–Planck equation associated with this problem acquires the form (compare Sec. XII.B),

$$\dot{f}=L_0 f+L_1 f, \tag{11.34}$$

where the operators L_0, L_1 are defined by

$$L_0=\sum_j\left[\frac{\partial}{\partial p_j}\frac{\partial H}{\partial q_j}-\frac{\partial}{\partial q_j}\frac{\partial H}{\partial p_j}\right]\equiv\sum_j\left[\frac{\partial H}{\partial q_j}\frac{\partial}{\partial p_j}-\frac{\partial H}{\partial p_j}\frac{\partial}{\partial q_j}\right] \tag{11.35}$$

and

$$L_1=\sum_j \gamma_j(\partial/\partial p_j)\left(p_j+m_jk_BT_j\frac{\partial}{\partial p_j}\right). \tag{11.36}$$

We focus our attention on the "unperturbed problem"

$$L_0 f_0=0, \tag{11.37}$$

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[26] This problem has been dealt with by many authors, e.g., Cox (1955) and Lebowitz and P. G. Bergmann (1957). We have chosen this model to demonstrate the basic ideas of our general method of solution.

and discuss the manifold of its solutions f_0. Because the right-hand side of Eq. (11.35) is the Poisson bracket with the Hamilton function, the solutions of (11.37) are given by constants of motion of the unperturbed problem:

$$h_1(p,q),\cdots,h_M(p,q). \tag{11.38}$$

We assume that the set (11.38) is irreducible in the sense that no one of these functions can be expressed as a function of the other ones.

We discuss the number M of constants of motion. Naively considered, the answer could be as follows. For N degrees of freedom, we have $2N$ initial values q_j^0, p_j^0, on which the solutions of the equations of motion depend. Thus

$$q_j = q_j(\mathbf{q}^0, t), \tag{11.39}$$

$$p_j = p_j(\mathbf{q}^0, t). \tag{11.40}$$

Elimination of time t leads us to $2N-1$ relations $g_l(\mathbf{q},\mathbf{p};\mathbf{q}^0,\mathbf{p}^0)\,(=g_l)$ which may be considered as constants of motion. Thus we expect $2N-1$ constants of motion. This conclusion is wrong, however, as is well known in the statistical mechanics community. The reason is that: the elimination of t requires that one of the relations (11.39) or (11.40) be inverted. This is in general not possible, however, because

$$t = t(p,q;p^0,q^0) \tag{11.41}$$

cannot be determined uniquely where t is a multivalued function (think of Lissajou's figures!). In general there exist only very few constants of motion, $M \ll 2N$. In many practical cases, M is of the order of unity. The basic idea in solving the *total* Fokker–Planck equation is this: Any function of $h_1,\cdots,h_M$:

$$f_0(h_1,\cdots,h_M) \tag{11.42}$$

is a solution of Eq. (11.37). Thus the unperturbed problem (11.37) is highly degenerate. This degeneracy will be lifted by the application of L_1 (11.36). We determine the resulting f_0 in the limit $\gamma_j \to 0$. We now formulate the problem in an abstract way:

2. The general case: Time-independent solution

We describe the system by coordinates $q_1,\cdots,q_N$ (where q may also stand for momenta!). Let L_0 be a linear operator depending on $q_1,\cdots,q_N$ and its derivatives (we admit even higher-order derivatives) or an integral operator which has the following property: If Eq. (11.37) is fulfilled by a set of functions $h_1,\cdots,h_M$, then an arbitrary function (11.42) is again a solution of (11.37). We assume L_1 in the form

$$L_1 = \sum_j (\partial/\partial q_j) l_j(q) + \sum_{ij} (\partial/\partial q_i) Q_{ij}(q) (\partial/\partial q_j) \tag{11.43}$$

though later on it will become obvious that our general procedure applies also to operators L_1 which contain higher-order derivatives (q without index stands for $q_1,\cdots,q_N$). Though we do not treat the process of non-Markovian heatbaths explicitly, our procedure applies to those heatbaths as well.

We treat L_1 as a perturbation, where the solutions of the unperturbed system are given by $f_0(h_1,\cdots,h_M)$. In order to perform the perturbation theory with respect to the degenerate system we must require that $L_1 f_0$ vanishes in the subspace spanned by all solutions of Eq. (11.37), i.e.,

$$\int g(h_1(q),\cdots,h_M(q)) L_1 f_0(h_1(q),\cdots,h_M(q))\, d^N q = 0, \tag{11.44}$$

where g is an arbitrary function. The integration volume is abbreviated by

$$d^N q = dq_1\cdots dq_N. \tag{11.45}$$

Performing the differentiations in Eq. (11.44), according to (11.43) we obtain

$$\begin{aligned} L_1 f_0 = {} & \sum_j \frac{\partial l_j(q)}{\partial q_j}\cdot f_0 + \sum_j l_j(q) \sum_\mu \frac{\partial f_0}{\partial h_\mu}\frac{\partial h_\mu(q)}{\partial q_j} \\ & + \sum_{ij} \frac{\partial Q_{ij}}{\partial q_i} \sum_\mu \frac{\partial f_0}{\partial h_\mu}\frac{\partial h_\mu(q)}{\partial q_j} \\ & + \sum_{ij} Q_{ij} \left(\sum_\mu \frac{\partial^2 h_\mu(q)}{\partial q_i \partial q_j}\frac{\partial f_0}{\partial h_\mu} + \sum_{\mu\nu} \frac{\partial h_\mu(q)}{\partial q_i}\frac{\partial h_\nu(q)}{\partial q_j}\frac{\partial^2 f}{\partial h_\mu \partial h_\nu}\right), \end{aligned} \tag{11.46}$$

where $\mu,\nu = 1,\cdots,M;\ j,i = 1,\cdots,N$. It is apparent that (11.46) can be written in a more concise form as

$$L_1\left(q,\frac{\partial}{\partial q}\right) f_0(h_1(q),\cdots,h_M(q)) = \tilde{L}_1\left(q,\frac{\partial}{\partial h}\right) f_0(h_1,\cdots,h_M). \tag{11.47}$$

We now introduce a product of δ functions in the following way which leaves Eq. (11.44) unchanged in mathematical content

$$\begin{aligned} & \int\!\!\int g(h_1,\cdots,h_M) \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q)) \tilde{L}_1(q,\partial/\partial h) \\ & \quad \times f_0(h_1,\cdots,h_M)\, d^N q\, d^M h = 0. \end{aligned} \tag{11.48}$$

Because g is an arbitrary function in the space spanned by the variables $h_1,\cdots,h_M$, Eq. (11.48) is only fulfilled if

$$\underbrace{\left\{ \int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q)) \tilde{L}_1\left(q,\frac{\partial}{\partial h}\right) d^N q \right\}}_{\hat{L}_1(h)} f_0(h_1,\cdots,h_M) = 0 \tag{11.49}$$

holds. Equation (11.49) reads explicitly

$$\begin{aligned} \hat{L}_1 f_0(h) = {} & a(h) f_0 + \sum_\mu b^{(\mu)}(h) (\partial f_0/\partial h_\mu) \\ & + \sum_{\mu\nu} c^{(\mu,\nu)} (\partial^2 f_0/\partial h_\mu \partial h_\nu) = 0, \end{aligned} \tag{11.50}$$

where we define the transform T by

$$T(\varphi(q)) = \int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q))\varphi(q)\, d^N q, \tag{11.51}$$

and

$$a(h) = \sum_j T(\partial l_j(q)/\partial q_j), \tag{11.52}$$

$$b^{(\mu)}(h) = \sum_j T\left(l_j(q)\, \frac{\partial h_\mu(q)}{\partial q_j}\right) + \sum_j T\left(\frac{\partial}{\partial q_i}\left(Q_{ij}\, \frac{\partial h_\mu}{\partial q_j}\right)\right), \tag{11.53}$$

$$c^{(\mu,\nu)}(h) = \sum_{ij} T\left(Q_{ij}\, \frac{\partial h_\mu}{\partial q_i}\, \frac{\partial h_\nu}{\partial q_j}\right). \tag{11.54}$$

Equation (11.50) can be cast into a more elegant form if we assume that we may perform partial integrations in the integrals (11.52) and (11.53). Inserting the explicit form of (11.47) into (11.49) the following quantities occur

$$\int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q)) l_j(q)\, \frac{\partial h_\mu(q)}{\partial q_j}\, d^N q = G_j^{\mu}(h), \tag{11.55}$$

$$\int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q))\, \frac{\partial l_j(q)}{\partial q_j}\, d^N q = \sum_\mu \frac{\partial}{\partial h_\mu} G_j^{\mu}(h), \tag{11.56}$$

$$\int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q)) Q_{ij}(q)\, \frac{\partial h_\mu(q)}{\partial q_i}\, \frac{\partial h_\nu(q)}{\partial q_j}\, d^N q = G_{ij}^{\mu\nu}, \tag{11.57}$$

$$\begin{aligned}\int \prod_{\lambda=1}^{M} \delta(h_\lambda - h_\lambda(q)) &\left\{\frac{\partial Q_{ij}}{\partial q_i}\, \frac{\partial h_\mu(q)}{\partial q_j} + Q_{ij}\, \frac{\partial^2 h_\mu}{\partial q_i\, \partial q_j}\right\} d^N q \\ &= \sum_\nu \int \prod_{\lambda \neq \nu} \delta(h_\lambda - h_\lambda(q))\, \frac{\partial}{\partial h_\nu}\, \delta(h_\nu - h_\nu(q)) \\ &\quad \times \frac{\partial h_\nu}{\partial q_i}\, Q_{ij}\, \frac{\partial h_\mu(q)}{\partial q_j}\, d^N q \\ &= \sum_\nu \frac{\partial}{\partial h_\nu} G_{ij}^{\mu\nu}.\end{aligned} \tag{11.58}$$

Equation (11.49) acquires the form

$$\hat{L} f_0(h_1, \cdots, h_M) = \sum_\mu \frac{\partial}{\partial h_\mu} (G^\mu f_0) + \sum_{\mu\nu} \frac{\partial}{\partial h_\nu}\left(G^{\mu\nu}\, \frac{\partial}{\partial h_\mu} f_0\right) = 0 \tag{11.59a}$$

where

$$G^\mu = \sum_j G_j^\mu \qquad \text{and} \qquad G^{\mu\nu} = \sum_{ij} G_{ij}^{\mu\nu}. \tag{11.59b}$$

This is our main result. It demonstrates that the problem of solving the high-dimensional Fokker–Planck equation (11.34) $\dot{f} = 0$, with L_0 representing a broad class of Liouville operators and with L_1 given by Eq. (11.43), can be reduced to solving a Fokker–Planck equation whose dimension is given by the number of relevant constants of motion.

3. Examples for the application of Eq. (11.59)

In order to demonstrate its usefulness and to show that this method leads to nontrivial results, we treat a case in which the dynamical system described by L_0 has only one relevant constant of motion (for instance the Hamiltonian). Then Eq. (11.59) reduces to the one-dimensional Fokker–Planck equation

$$\frac{\partial}{\partial h}\left(\left(\sum_j G_j + \sum_{ij} G_{ij}\, \frac{\partial}{\partial h}\right) f_0\right) = 0, \tag{11.60}$$

where

$$G_j^{\mu} = G_j, \qquad G_{ij}^{\mu\nu} = G_{ij}. \tag{11.61}$$

Taking into account the boundary conditions, the general solution of Eq. (11.60) reads

$$f_0 = N \exp\left\{-\int^h \left(\sum_j G_j / \sum_{ij} G_{ij}\right) dh\right\}, \tag{11.62}$$

where N is a normalization constant. In order to elucidate the content of both Eq. (11.62) and Eq. (11.59) we now treat the problem described in (11.34), (11.35), (11.36).

A system of interacting particles. Here we assume h in the form

$$h = H = \sum p_j^2/2m_j + V(q_1, q_2, \cdots). \tag{11.63}$$

We further adopt the attitude of statistical mechanics: We assume that h is in the present case the only constant of motion. G_j and G_{ij} [compare Eqs. (11.61) and (11.36)] are now defined by

$$G_j = \int \delta(H - H(p, q)) \gamma_j p_j (\partial H/\partial p_j)\, d^N p\, d^N q \tag{11.64}$$

and

$$G_{ij} = \int \delta(H - H(p, q)) \delta_{ij} \gamma_j m_j k_B T_j (\partial H/\partial p_j)^2\, d^N p\, d^N q \tag{11.65}$$

Inserting Eq. (11.63) into (11.64) and (11.65), both integrals have the same form apart from different numerical factors:

$$G_j \propto G_{jj} \propto \int \delta\left(H - \sum p_j^2/2m_j - V(q)\right) p_j^2/m_j\, d^N q\, d^N q. \tag{11.66}$$

Making the replacement

$$p_j^2/m_j = \xi_j, \tag{11.66a}$$

one immediately realizes that the integral (11.66) is independent of the index j. With this in mind we obtain instead of formula (11.62)

$$f = N \exp[-\beta_{\text{eff}} H(p, q)], \tag{11.67}$$

where the effective temperature T_{eff} is now defined by

$$\frac{1}{k_B T_{\text{eff}}} \equiv \beta_{\text{eff}} = \sum_j \gamma_j \Big/ \sum_j \gamma_j k_B T_j. \tag{11.68}$$

In contrast to equilibrium systems, the distribution function now depends explicitly on the damping constants γ_j. If all temperatures are equal, Eq. (11.67) reduces to the well-known Boltzman distribution function.

Further examples have been found in laser theory [Haken and Wöhrstein (1973)] and in nonlinear optics [Haken (1973d)]. The relevant conservation laws are discussed in Secs. III and IV of our present article.

4. Time-dependent solutions

We show that our above method can be extended to the time-dependent case, at least under certain conditions. We still assume that L_0 is time independent and has the same properties as above, but we admit a time-dependent L_1: $L_1(t)$. The class of solutions of the unperturbed problem

$$L_0 f^{(0)} = df^{(0)}/dt \tag{11.69}$$

comprises (11.42), but also time-dependent distribution functions. We treat as an example

$$L_0 = -\sum_{\nu=1}^{N} \frac{\partial}{\partial q_\nu} (k_\nu(q)\cdots), \tag{11.70}$$

with

$$\sum_{\nu=1}^{N} \frac{\partial k_\nu}{\partial q_\nu} = 0. \tag{11.71}$$

Imposing the initial condition

$$f^{(0)}(q;0) = \prod_{\nu=1}^{N} \delta(q_\nu - q_\nu^0), \tag{11.72}$$

$f^{(0)}$ is given by

$$f^{(0)}(q;t) = \prod_{\nu=1}^{N} \delta(q_\nu - q_\nu(t)). \tag{11.73}$$

Here $q_\nu(t)$ are the solutions of the equations of motion

$$\dot{q}_\nu(t) = k_\nu(q(t)) \tag{11.74}$$

subject to the initial conditions

$$q_\nu(0) = q_\nu^{(0)}. \tag{11.75}$$

The manifold of solutions (11.73) is, of course, bigger than (11.42). Thus, even in the unperturbed case, we cannot treat the fully time-dependent problem only by means of (11.42). The situation changes, however, if we admit as initial distribution only those of the form (11.42). If furthermore L_1 is small and changes slowly enough, we may extend our result (11.59) to

$$\dot{f}_0(h_1,\cdots,h_M;t) = \sum_\mu \frac{\partial}{\partial h_\mu}(G^\mu(t) f_0) + \sum_{\mu\nu} \frac{\partial}{\partial h_\nu}\left(G^{\mu\nu}(t) \frac{\partial}{\partial h_\mu} f_0\right) \tag{11.76}$$

where the G's are defined in Eqs. (11.55) and (11.57).

5. Continuously many variables

Fokker–Planck equations may also be formulated for systems described by continuously many variables. Consider as an example the i component of the electric field strength, $E_i(x)$. We adopt the following notation. We replace both the continuous space coordinate x and the discrete variable i quite generally by a variable s and write $q(s)$ instead of $E_i(x)$:

$$\begin{aligned} &i, x \to s, \\ &E_i(x) \to q(s). \end{aligned} \tag{11.77}$$

We write L_1 in the form

$$L_1 = \int \frac{\delta}{\delta q(s)} l(q,s)\, ds + \iint \frac{\delta^2}{\delta q(s)\delta q(s')} \times Q(q,s,s')\, ds\, ds' \tag{11.78}$$

which incidentally may serve as an explicit example of the structure of L_0. Here l and Q may be functionals of $q(s)$. We assume that the relevant solutions of Eq. (11.37) are spanned by the basic set of relevant functions $h_1,(q)\cdots$, $h_n(q)$, where

$$h_j(\{q(s)\}) \tag{11.79}$$

is a functional of the functions $q(s)$. A straightforward analysis leads to the final Fokker–Planck equation (11.59) with the following definitions

$$G^\mu = \int G^\mu(s)\, ds; \qquad G^{\mu\nu} = \iint G^{\mu\nu}(s,s')\, ds\, ds', \tag{11.80}$$

$$G^\mu(s) \equiv G^\mu(h,s) = \int \prod_{\lambda=1}^{n} \delta(h_\lambda - h_\lambda(q)) l(q,s) \frac{\delta h_\mu(q)}{\delta q(s)} Dq, \tag{11.81}$$

$$G^{\mu\nu}(h,s,s') = \int \prod_{\lambda=1}^{n} \delta(h_\lambda - h_\lambda(q)) Q(q,s,s') \frac{\delta h_\nu(q)}{\delta q(s)} \frac{\delta h_\mu(q)}{\delta q(s')} Dq. \tag{11.82}$$

where Dq denotes functional integration.

D. Exact stationary solution of the Fokker-Planck equation for systems in detailed balance

In this section we mainly demonstrate two things [Graham and Haken (1971a), Risken (1972)]:

(1) We derive sufficient and necessary conditions for the drift and diffusion coefficients of the Fokker–Planck equation so that the principle of detailed balance is fulfilled.

(2) We show that under the condition of detailed balance the stationary solution of the Fokker–Planck equation may be found explicitly by quadratures.

While the principle of detailed balance is expected to hold for practically all systems in thermal equilibrium, this need not be so in systems far from thermal equilibrium. Thus each individual case requires a detailed discussion (e.g., by symmetry considerations) if this principle is applicable. Also the inspection of the structure of the Fokker–Planck equation will enable us (see below), to decide whether detailed balance is present.

1. Detailed balance

We denote the set of variables $q_1, \cdots, q_N$ by $\mathbf{q}$ and the set of the variables under time reversal by

$$\tilde{\mathbf{q}} = \{\epsilon_1 q_1, \cdots, \epsilon_N q_N\}, \tag{11.83}$$

where $\epsilon_i = -1$ $(+1)$ depending on whether the coordinate q_i changes sign (does not change sign) under time reversal, and $\boldsymbol{\lambda}$ stands for a set of externally determined parameters. The time reversed quantity is denoted by

$$\tilde{\boldsymbol{\lambda}} = \{\nu_1 \lambda_1, \cdots, \nu_M \lambda_M\}, \tag{11.84}$$

where $\nu_i = -1$ $(+1)$ depends on the inversion symmetry of the external parameters under time reversal. We denote the joint probability of finding the system at t_1 with coordinates $\mathbf{q}$ and at t_2 with coordinates $\mathbf{q}'$ by (see Eq. 10.21))

$$f_2(\mathbf{q}', \mathbf{q}, t_2, t_1). \tag{11.85}$$

In the following we consider a stationary system so that the joint probability depends only on the time difference $t_2 - t_1 = \tau$. Thus (11.85) may be written as

$$f_2(\mathbf{q}', \mathbf{q}; t_2, t_1) = W(\mathbf{q}', \mathbf{q}; \tau). \tag{11.86}$$

We now formulate the principle of detailed balance. There are two definitions available:

(1) *The principle of detailed balance* (*first version*). [See e.g., de Groot and Mazur (1961)]. It reads

$$W(\mathbf{q}', \mathbf{q}, \tau; \boldsymbol{\lambda}) = W(\tilde{\mathbf{q}}, \tilde{\mathbf{q}}', \tau; \tilde{\boldsymbol{\lambda}}). \tag{11.87}$$

Because the joint probability may be expressed by the stationary distribution $f(\mathbf{q})$ multiplied by the conditional probability p [compare Eq. (10.30)], where we now write

$P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda})$ instead of $p_{t't}(\mathbf{q}', \mathbf{q})$,

we may reformulate Eq. (11.87) as follows

$$P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda}) f(\mathbf{q}, \boldsymbol{\lambda}) = P(\tilde{\mathbf{q}} \mid \tilde{\mathbf{q}}'; \tau, \tilde{\boldsymbol{\lambda}}) f(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}). \tag{11.88}$$

Here and in the following we assume that the Fokker–Planck equation possesses a unique stationary solution. One may then show directly that

$$f(\mathbf{q}, \boldsymbol{\lambda}) = f(\tilde{\mathbf{q}}, \tilde{\boldsymbol{\lambda}}) \tag{11.89}$$

holds. We define the transition probability per second by

$$w(\mathbf{q}', \mathbf{q}; \boldsymbol{\lambda}) = [(d/d\tau) P(\mathbf{q}' \mid \mathbf{q}; \tau; \boldsymbol{\lambda})]_{\tau=0}. \tag{11.90}$$

Taking the derivative with respect to τ on both sides of Eq. (11.88) and putting $\tau = 0$ (but $\mathbf{q} \neq \mathbf{q}'$) we obtain

(2) *the condition of detailed balance* (*second version*)

$$w(\mathbf{q}', \mathbf{q}; \boldsymbol{\lambda}) f(\mathbf{q}, \boldsymbol{\lambda}) = w(\tilde{\mathbf{q}}, \tilde{\mathbf{q}}'; \tilde{\boldsymbol{\lambda}}) f(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}). \tag{11.91}$$

It has obviously a very simple meaning. The left-hand side describes the total transition rate out of the state $\mathbf{q}$ into a new state $\mathbf{q}'$. The principle of detailed balance then requires that this transition rate is equal to the rate in the reverse direction for $\mathbf{q}'$ and $\mathbf{q}$ with reverse motion e.g. with reverse momenta.

2. The required structure of the Fokker–Planck equation and its stationary solution

We now derive necessary and sufficient conditions on the form of a Fokker–Planck equation so that the principle of detailed balance in its second (and first) version are satisfied. Using the conditional probability P (which is nothing but the Green's function) we write the Fokker–Planck equation (or generalized Fokker–Planck equation having infinitely many derivatives) in the form of the equation

$$\frac{d}{d\tau} P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda}) = L(\mathbf{q}', \boldsymbol{\lambda}) P(\mathbf{q}' \mid \mathbf{q}; \tau; \lambda). \tag{11.92}$$

Note that, if not otherwise stated, L may also be an integral operator. The solution of Eq. (11.92) is subject to the initial condition

$$P(\mathbf{q}' \mid \mathbf{q}; 0, \boldsymbol{\lambda}) = \delta(\mathbf{q}' - \mathbf{q}). \tag{11.93}$$

The formal solution of Eq. (11.92) with (11.93) reads

$$P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda}) = \exp[L(\mathbf{q}', \boldsymbol{\lambda}) \tau] \delta(\mathbf{q}' - \mathbf{q}). \tag{11.92a}$$

Putting into (11.92) on both sides $\tau = 0$, (11.92) acquires the form

$$w(\mathbf{q}', \mathbf{q}; \boldsymbol{\lambda}) = L(\mathbf{q}', \boldsymbol{\lambda}) \delta(\mathbf{q}' - \mathbf{q}). \tag{11.94}$$

The backward equation (backward Kolmogorov equation) is defined by

$$(d/d\tau) P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda}) = L^+(\mathbf{q}, \boldsymbol{\lambda}) P(\mathbf{q}' \mid \mathbf{q}; \tau, \boldsymbol{\lambda}), \tag{11.95}$$

where L^+ is the operator adjoint to L. Again specializing Eq. (11.95) for $\tau = 0$ we obtain

$$w(\mathbf{q}', \mathbf{q}; \boldsymbol{\lambda}) = L^+(\mathbf{q}, \boldsymbol{\lambda}) \delta(\mathbf{q}' - \mathbf{q}). \tag{11.96}$$

Proceeding in Eq. (11.96) to time-inverted coordinates and then inserting Eqs. (11.94) and (11.96) into (11.91) we obtain

$$L(\mathbf{q}', \boldsymbol{\lambda}) \delta(\mathbf{q}' - \mathbf{q}) f(\mathbf{q}, \boldsymbol{\lambda}) = L^+(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}) \delta(\tilde{\mathbf{q}}' - \tilde{\mathbf{q}}) f(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}). \tag{11.97}$$

We now demonstrate how one may derive an operator identity to be fulfilled by L, L^+ which is a consequence of Eq. (11.97). On the left-hand side of Eq. (11.97) we replace $\mathbf{q}$ by $\mathbf{q}'$ in f. On the right-hand side we make the replacement

$$\delta(\tilde{\mathbf{q}}' - \tilde{\mathbf{q}}) = \delta(\mathbf{q}' - \mathbf{q}). \tag{11.98}$$

With these substitutions and bringing the right-hand side to the left-hand side, Eq. (11.97) acquires the form

$$L(\mathbf{q}', \boldsymbol{\lambda}) f(\mathbf{q}', \boldsymbol{\lambda}) \delta(\mathbf{q}' - \mathbf{q}) - f(\mathbf{q}', \boldsymbol{\lambda}) L^+(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}) \delta(\mathbf{q}' - \mathbf{q}) = 0. \tag{11.99}$$

Because the δ function is an arbitrary function if we let $\mathbf{q}$ accept all values, Eq. (11.99) is equivalent to the following operator equation [(Risken (1972)]

$$L(\mathbf{q}', \boldsymbol{\lambda}) f(\mathbf{q}', \boldsymbol{\lambda}) - f(\mathbf{q}', \boldsymbol{\lambda}) L^+(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}) = 0. \tag{11.100}$$

In Eq. (11.100) L acts in the usual sense of an operator well known from quantum mechanical operators so that Lf is to be interpreted as $L(f\cdots)$ where the points indicate an arbitrary function. So far we have seen that the condition of detailed balance has the consequence (11.100).

We now demonstrate that if Eq. (11.100) is fulfilled the system even has the property of the first version principle of detailed balance (which appears to be stronger). First we note that Eq. (11.100) may be iterated yielding

$$(L(\mathbf{q}', \boldsymbol{\lambda}))^n f(\mathbf{q}', \boldsymbol{\lambda}) = f(\mathbf{q}', \boldsymbol{\lambda}) (L^+(\tilde{\mathbf{q}}', \tilde{\boldsymbol{\lambda}}))^n. \tag{11.101}$$

We multiply Eq. (11.101) by $\tau^n(1/n!)$ and sum up over n from $n = 0$ to $n = \infty$. Now making all steps which have led from Eq. (11.97) to Eq. (11.100) in the reverse direction, and using Eq. (11.92a) and its analogous form for L^+ we obtain Eq. (11.88) and thus Eq. (11.87). We now exploit (11.100) to determine the explicit form of the Fokker–Planck equation if the system fulfills the condition of detailed balance. Because (11.100) is an operator identity each coefficient of all derivatives with respect to q_i must vanish. Though in principle the comparison of coeficients is possible for arbitrarily high derivatives, we confine ourselves to the usual Fokker–Planck equation with an operator L of the form

$$L(q) = -\sum_i (\partial/\partial q_i) \cdot K_i(\mathbf{q}, \boldsymbol{\lambda}) + \tfrac{1}{2} \sum_{ik} (\partial^2/\partial q_i\, \partial q_k) \times K_{ik}(\mathbf{q}, \boldsymbol{\lambda}). \tag{11.102}$$

and its adjoint

$$L^+(\mathbf{q}) = \sum_i K_i(\mathbf{q}, \boldsymbol{\lambda}) (\partial/\partial q_i) + \tfrac{1}{2} \sum_{ik} K_{ik}(\mathbf{q}, \boldsymbol{\lambda}) \times (\partial^2/\partial q_i\, \partial q_k). \tag{11.103}$$

We always may assume that the diffusion coefficients are symmetric

$$K_{ik} = K_{ki}. \tag{11.104}$$

It is convenient to define the following new coefficients:

(a) the irreversible drift coefficients

$$D_i(\mathbf{q}, \boldsymbol{\lambda}) = \tfrac{1}{2}(K_i(\mathbf{q}, \boldsymbol{\lambda}) + \epsilon_i K_i(\tilde{\mathbf{q}}, \tilde{\boldsymbol{\lambda}})) \equiv D_i^{ir} \tag{11.105}$$

(b) the reversible drift coefficients

$$J_i(\mathbf{q}, \boldsymbol{\lambda}) = \tfrac{1}{2}(K_i(\mathbf{q}, \boldsymbol{\lambda}) - \epsilon_i K_i(\tilde{\mathbf{q}}, \tilde{\boldsymbol{\lambda}})) \equiv D_i^{r}. \tag{11.106}$$

For applications it is important to note that J_i transforms as $\dot{q}_i$ under time reversal. We then obtain explicitly the *necessary and sufficient conditions for* K_{ik}, D_i *and* J_i *so that the principle of detailed balance holds.* (*Graham and Haken* (1971a)).[27] We write the stationary solution of the Fokker–Planck equation in the form

$$f(\mathbf{q}, \boldsymbol{\lambda}) = N \exp[-\phi(\mathbf{q}, \boldsymbol{\lambda})], \tag{11.107}$$

where N is the normalization constant and ϕ may be interpreted as a generalized thermodynamic potential. The conditions read

$$K_{ik}(\mathbf{q}, \boldsymbol{\lambda}) = \epsilon_i \epsilon_k K_{ik}(\tilde{\mathbf{q}}, \tilde{\boldsymbol{\lambda}}), \tag{11.108}$$

$$D_i - \tfrac{1}{2} \sum_k \frac{\partial K_{ik}}{\partial q_k} = -\tfrac{1}{2} \sum_k K_{ik} \frac{\partial \phi}{\partial q_k}, \tag{11.109}$$

$$\sum_i \left(\frac{\partial J_i}{\partial q_i} - J_i \frac{\partial \phi}{\partial q_i} \right) = 0. \tag{11.110}$$

If the diffusion matrix K possesses an inverse, (11.109) may be solved with respect to the gradient of ϕ

$$\frac{\partial \phi}{\partial q_i} = \sum_k (K^{-1})_{ik} \left(\sum_l \frac{\partial K_{kl}}{\partial q_l} - 2D_k \right) \equiv A_i. \tag{11.111}$$

This shows that (11.109) implies the integrability condition

$$(\partial/\partial q_j) A_i = (\partial/\partial q_i) A_j \tag{11.112}$$

which is a condition on the drift and diffusion coefficients as defined by the right-hand side of Eq. (11.111). Substituting A_i, A_j by Eq. (11.111), the condition (11.110) acquires the form

$$\sum_i \left[\frac{\partial J_i}{\partial q_i} - J_i \sum_k (K^{-1})_{ik} \left(\sum_l \frac{\partial K_{kl}}{\partial q_l} - 2D_k \right) \right] = 0. \tag{11.113}$$

Thus the conditions that detailed balance holds are given finally by Eqs. (11.108), (11.112), and (11.113). Equation (11.109) or equivalently (11.111) then allows us to determine ϕ by pure quadratures, i.e., by a line integral. *Thus the stationary solution of the Fokker–Planck equation may be determined explicitly* (The deeper reason for these results will become more obvious in Sec. XI.E.)

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[27] The conditions (11.108)–(11.109) had been previously derived by van Kampen (1957) and Uhlborn (1960) in a somewhat different manner. We wish to thank a referee for drawing our attention to these two references.

3. Useful special cases

We mention two special cases which have turned out to be extremely useful for applications.

(1) $J_i = 0$ yields the so-called potential conditions (Stratonovich (1963)) in which case (11.110) and thus (11.113) are fulfilled identically so that only (11.108) and (11.112) remain to be satisfied.

(2) In many practical applications one deals with complex variables (instead of the real ones)[28] and the Fokker–Planck equation has the following explicit form

$$\frac{\partial f}{\partial t} = \left\{ \sum_j \left(\frac{\partial}{\partial u_j} C_j + \frac{\partial}{\partial u_j^*} \tilde{C}_j \right) + \sum_{kj} Q_{kj} \frac{\partial^2}{\partial u_k \, \partial u_j^*} \right\} f \tag{11.114}$$

with

$$Q_{kj} = \delta_{kj} Q_j, \qquad Q_j = Q. \tag{11.115}$$

Then the above conditions reduce to the following ones (Haken (1969a)): C_j, $\tilde{C}_j$ must have the form

$$C_j = \partial B / \partial u_j^* + I_j^{(1)}, \tag{11.116}$$

$$\tilde{C}_j = \partial B / \partial u_j + I_j^{(2)}, \tag{11.117}$$

and the following conditions must be satisfied

$$\sum_j \left(\frac{\partial B}{\partial u_j} I_j^{(1)} + \frac{\partial B}{\partial u_j^*} I_j^{(2)} \right) = 0, \tag{11.118}$$

$$\sum_j \left(\frac{\partial I_j^{(1)}}{\partial u_j} + \frac{\partial I_j^{(2)}}{\partial u_j^*} \right) = 0. \tag{11.119}$$

As a result the stationary solution of Eq. (11.114) reads

$$f = N e^{-\phi}, \tag{11.120}$$

where

$$\phi = 2B/Q. \tag{11.120a}$$

E. Exact stationary solution of the master equation for systems far from thermal equilibrium in detailed balance

In this section we start directly from the master equation and prove the following: If the master equation [Landauer (1962), Haken (1974a)] has a unique stationary solution and fulfills the principle of detailed balance, this solution can be obtained explicitly by mere summations or, in the continuous case, by quadratures.

We denote by $\mathbf{m}$ (or $\mathbf{n}$) a set of variables $(m_1, \cdots, m_N)$. Here λ denotes a set of external parameters. The transition probability per second from state $\mathbf{m}$ to $\mathbf{n}$ under the influence of λ is denoted by $w(\mathbf{n}, \mathbf{m}; \lambda)$. The distribution function is denoted by $f(\mathbf{n}, \lambda)$. The master equation then reads (compare Eq. (10.37)

$$\dot{f}(\mathbf{n}; \lambda) = \sum_{\mathbf{m}} w(\mathbf{n}, \mathbf{m}; \lambda) f(\mathbf{m}, \lambda) - f(\mathbf{n}, \lambda) \sum_{\mathbf{m}} w(\mathbf{m}, \mathbf{n}; \lambda). \tag{11.121}$$

Putting $\dot{f} = 0$ we consider the stationary state. We introduce the time reversed variables by

$$\tilde{\mathbf{n}} = (\epsilon_1 n_1, \cdots, \epsilon_N n_N), \tag{11.122}$$

where $\epsilon_1 = +1$ (-1) if the variables are even (odd) under time reversal. We use a similar notation for λ. Then the principle of detailed balance requires that

$$w(\mathbf{n}, \mathbf{m}; \lambda) f(\mathbf{m}, \lambda) = w(\tilde{\mathbf{m}}, \tilde{\mathbf{n}}; \lambda) f(\mathbf{n}, \tilde{\lambda}) \tag{11.123}$$

is fulfilled.

Equation (11.123) represents a set of homogeneous equations, which can be solved only if certain conditions are fulfilled by the w's. Such conditions can be derived, for instance, by symmetry considerations or in the case that w can be replaced by differential operators. We are not concerned, however, with this question, but want to show how Eq. (11.123) leads to an explicit solution. In the following we assume that $f(\mathbf{n}; \lambda) \neq 0$. Then Eq. (11.123) can be written as

$$\frac{f(\mathbf{m}; \lambda)}{f(\mathbf{n}; \lambda)} = \frac{w(\tilde{\mathbf{m}}, \tilde{\mathbf{n}}; \tilde{\lambda})}{w(\mathbf{n}, \mathbf{m}; \lambda)}. \tag{11.124}$$

Writing $\mathbf{m} = \mathbf{n}_{j+1}$, $\mathbf{n} = \mathbf{n}_j$, we pass from $\mathbf{n}_0$ to $\mathbf{n}_N$ by a chain of intermediate states. Because there exists a unique solution, at least one chain must exist. We then find

$$\frac{f(\mathbf{n}_N, \lambda)}{f(\mathbf{n}_0, \lambda)} = \prod_{j=0}^{N-1} \frac{w(\tilde{\mathbf{n}}_{j+1}, \tilde{\mathbf{n}}_j, \tilde{\lambda})}{w(\mathbf{n}_j, \mathbf{n}_{j+1}, \lambda)}. \tag{11.125}$$

Equation (11.125) generalizes a result obtained by Landauer (1962) (one variable and nearest-neighbor transitions) to an arbitrary number of dimensions and arbitrary transitions. Putting

$$f(\mathbf{m}, \lambda) = N \exp \phi(\mathbf{m}, \lambda), \tag{11.126}$$

where N is the normalization factor, Eq. (11.125) may be written as

$$\phi(\mathbf{n}_N, \lambda) - \phi(\mathbf{n}_0, \lambda) = \sum_{j=0}^{N-1} \ln \{ w(\tilde{\mathbf{n}}_{j+1}, \tilde{\mathbf{n}}_j; \tilde{\lambda}) / w(\mathbf{n}_j, \mathbf{n}_{j+1}; \lambda) \}. \tag{11.127}$$

Because the solution was assumed to be unique, $\phi(\mathbf{m}_N, \lambda)$ is independent of the path chosen. Taking a suitable limit one may apply Eq. (11.127) to continuous variables.

F. Exact and approximate relations between moments

We consider a Fokker–Planck equation or a generalized Fokker–Planck equation. We split the corresponding operators of the equation of motion into a part which refers to

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[28] To establish the connection between these variables, note that Re u is an even variable, whereas Im u is an odd one.

the proper system and another one which describes the coupling of the proper system to the external world (reservoirs). We demonstrate that by use of conservation laws [see Eqs. (11.37), (11.38)] referring to the proper systems, exact relations hold for certain moments, valid for all temperatures and coupling constants of the reservoirs [Haken (1973e)]. Using the concepts of Sec. XI.C we describe a perturbation theoretical approach which allows us in a simple manner to determine a number of important correlation functions (moments of the total system). We assume that the system is described by Eq. (11.34), where L_0 is the Liouville operator of the proper system. Here L_1 describes the coupling of the proper system to reservoirs. To exhibit the coupling strength explicitly, we extract from L_1 the parameter describing the strength of the coupling to the external world: $L_1 \longrightarrow \lambda L_1$. Thus our basic equation reads

$$\dot{f} = (L_0 + \lambda L_1) f. \tag{11.128}$$

We consider moments of the form

$$X_i = q_1^{n_1} \cdots q_M^{n_M}, \qquad i = \{n_1, \cdots, n_M\}. \tag{11.129}$$

We denote the operators adjoint to L_0, L_1 by $\hat{L}_0$, $\hat{L}_1$, respectively. We assume that the L's and $\hat{L}$'s respectively, may be represented by superpositions of derivatives with respect to q_i multiplied by superpositions of moments of the form (11.129). This restriction may easily be overcome by using more general functions instead of (11.129) as will become evident from what follows. We now form in obvious steps

$$\langle X_i L_0 f \rangle = \langle (\hat{L}_0 X_i) f \rangle = \sum_j C_{ij} \overline{X_j} \tag{11.130}$$

where the brackets denote the integration over all the variables, for which we have used the abbreviation

$$\overline{X_i} = \langle X_i f \rangle. \tag{11.131}$$

In a way analogous to Eq. (11.130) we find

$$\langle X_i L_1 f \rangle = \sum_j D_{ij} X_j. \tag{11.132}$$

We now multiply Eq. (11.128) from the left with X_i and take the average. This yields

$$(d/dt) \langle X_i f \rangle = \sum_j C_{ij} \overline{X_j} + \lambda \sum_j D_{ij} \overline{X_j}. \tag{11.133}$$

We now proceed to specialize this relation.

1. Time-independent relations ($\dot{f} = 0$)

a. Exact relations

We assume that L_0 is self-adjoint and assume that there exist constants of motion of the form

$$h_k = \sum_l E_{kl} X_l \tag{11.134}$$

so that

$$L_0 h_k = 0. \tag{11.135}$$

Multiplying Eq. (11.128) with (11.134) from the left and taking the average yields

$$\overline{h_k L_0} + \lambda \overline{h_k L_1} = 0 \tag{11.136}$$

where the first term vanishes. Expressing the second term by means of Eqs. (11.134) and (11.132) we find

$$\sum_j \overline{X_j} \sum_l E_{kl} D_{lj} = 0 \tag{11.137}$$

which gives a set of relations between the moments $\bar{X}_i$ which hold independently of the coupling strength λ of the proper system to reservoirs.

b. Perturbation approach

We now assume that λ is a small expansion parameter. We put the distribution function f in the form

$$f = f_0 + \lambda f_1 + \lambda^2 f_2 + \cdots. \tag{11.138}$$

If the unperturbed problem ($\lambda = 0$) is nondegenerate, Eq. (11.138) exists in a straightforward way. If it is degenerate the procedure of Sec. XI.C must be applied. According to the decomposition (11.138), there exists a corresponding decomposition of the moments

$$\begin{aligned} \langle X_j f \rangle &= \langle X_j f_0 \rangle + \lambda \langle X_j f_1 \rangle + \cdots \\ &\equiv \overline{X_j}^{(0)} + \lambda \overline{X_j}^{(1)} + \cdots. \end{aligned} \tag{11.139}$$

Inserting Eq. (11.139) into (11.133) yields, by a comparison of equal powers of λ, a recurrency relation of the form

$$\sum_j C_{ij} \overline{X_j}^{(k)} = - \sum_j D_{ij} \overline{X_j}^{(k-1)}. \tag{11.140}$$

Because the method of Sec. XI.C allows us to determine f_0, at least a number of correlation functions of the first order may be found.

2. Time-dependent relations

We only mention an example for which X_i is replaced by a constant of motion h_k.

$$(d/dt) \overline{h_k} = \sum_j \overline{X_j} \sum_l E_{kl} D_{lj} \tag{11.141}$$

Note, that on the right-hand side the matrix D_{lj} depends only on damping and diffusion constants, but no longer contains internal parameters of the proper system.

XII. GENERALIZED LANGEVIN EQUATIONS

A. Derivation of generalized Langevin equations

In many cases of practical interest we want to study the behavior of a certain system S which is coupled to reservoirs so that we ought to consider the total system $S + R$. On the other hand we are finally interested only in the behavior of the system S itself. This suggests that we find a formalism in which the variables of the system R are eventually eliminated. If we can describe the system $S + R$ by first-order differential equations we can achieve this in a rather simple manner. As a result we will find that the system R acts in three different ways on the system S:

(1) It brings about an additional interaction within the system S which may be considered to be instantaneous.

(2) It brings about a more or less retarded interaction which may give rise to a frictional force.

(3) On account of statistics inherent in the reservoir system there occur random forces in the proper system S.

For simplicity we assume that the reservoir system is composed of harmonic oscillators. It should be noted, however, that the derivation could be done more generally. Note that our analysis is not confined to physical systems. It may equally well apply, e.g., to electrical or neuron networks or other fields in the sense discussed in our article. We assume equations of motion of the proper system S in the form[29]

$$\dot{\mathbf{q}}(t) = \mathbf{K}(\mathbf{q}(t);t) + \mathsf{A}(\mathbf{q}(t);t)\mathbf{r}(t) \tag{12.1}$$

where $\mathbf{q}$ stands for a set of variables of the proper system, $\mathbf{r}$ for the reservoir variables, $\mathbf{K}$ may be a time-dependent "force," and A describes the strength of coupling to the reservoir coordinates $\mathbf{r}$. On the other hand we assume the equations of motion for the reservoirs in the form

$$\dot{\mathbf{r}}(t) = \mathsf{L}\mathbf{r}(t) - \mathbf{B}(\mathbf{q}(t)), \tag{12.2}$$

where L is a constant matrix and $\mathbf{B}$ may depend in an arbitrary manner on $\mathbf{q}$. We will assume that L possesses an inverse. If we let $\mathbf{q}$ stand for both coordinates and momenta and interpret $\mathbf{K}$ and $\mathsf{A}\,\mathbf{r}$ as suitable derivatives of a Hamiltonian, Eq. (12.1) contains as a special case the Hamiltonian equations of motion. Equation (12.2) possesses the solution

$$\mathbf{r}(t) = \exp(\mathsf{L}t)\mathbf{r}(0) - \int_0^t \exp[\mathsf{L}(t-\tau)]\mathbf{B}(\mathbf{q}(\tau))\,d\tau \tag{12.3}$$

which may be transformed by partial integration into[30]

$$\mathbf{r}(t) = \mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(t)) + \exp(\mathsf{L}t)\{\mathbf{r}(0) - \mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(0))\} - \int_0^t \exp[\mathsf{L}(t-\tau)]\mathsf{L}^{-1}\mathsf{C}(\mathbf{q}(\tau))\dot{\mathbf{q}}(\tau)\,d\tau \tag{12.4}$$

where we have introduced the matrix

$$\mathsf{C}(\mathbf{q}(\tau)) = (C_{lk}) = (\partial B_l/\partial q_k). \tag{12.5}$$

Inserting Eq. (12.4) into (12.1) yields the desired generalized Langevin equation

$$\begin{aligned}\dot{\mathbf{q}}(t) &= \mathbf{K}(\mathbf{q}(t);t) + \mathsf{A}(\mathbf{q}(t);t)\mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(t))\\ &\quad - \int_0^t \mathsf{A}(\mathbf{q}(t);t)\exp[\mathsf{L}(t-\tau)]\mathsf{L}^{-1}\mathsf{C}(\mathbf{q}(\tau))\dot{\mathbf{q}}(\tau)\,d\tau\\ &\quad + \mathsf{A}(\mathbf{q}(t);t)\exp\mathsf{L}t\,\{\mathbf{r}(0) - \mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(0))\}.\end{aligned} \tag{12.6}$$

The reservoir coordinates enter into it only through their initial value $\mathbf{r}(0)$. The first term on the right-hand side is the initially present force, the second term describes an instantaneous force brought about by the reservoirs. The integral describes a general retarded interaction and the last term may be interpreted as a fluctuation force. We regard the expression

$$\mathsf{F}(t) = \exp(\mathsf{L}t)\{\mathbf{r}(0) - \mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(0))\} \tag{12.7}$$

as the noise source. Its statistical properties depend on the statistical properties of $\mathbf{r}(0)$. We assume at time $t = 0$ the system R possesses a Gaussian distribution with mean values

$$\langle\mathbf{r}(0)\rangle = \mathsf{L}^{-1}\mathbf{B}(\mathbf{q}(0)). \tag{12.8}$$

Now with applications to physics in mind, we assume that the reservoir is composed of a set of physical systems each of which is kept at an individual temperature T_i. We assume that the matrix L may be decomposed into

$$\mathsf{L} = \begin{pmatrix} \mathsf{L}_1 & & & 0 \\ & \mathsf{L}_2 & & \\ & & \ddots & \\ 0 & & & \mathsf{L}_N \end{pmatrix}. \tag{12.9}$$

Incidentally we decompose $\mathbf{r}$ and F into the subvectors $\mathbf{r}_i$ and F_i, respectively, where $i = 1,\cdots,N$ corresponds to the indices of L in Eq. (12.9). Furthermore we assume that we may put

$$\mathsf{L}_i = \mathbf{z}_i\tilde{\mathsf{L}}_i, \tag{12.10}$$

where $\mathbf{z}_i$ is a direct product of antisymmetric matrices of the form

$$\mathbf{z} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{12.11}$$

which take care of the fact that the Hamiltonian equation carries two different signs with respect to the equations for coordinates and momenta, respectively. Here $\tilde{\mathsf{L}}_i$ is assumed to be symmetric and nonsingular. Assuming that the different reservoirs are uncorrelated we have

$$\langle\Delta\mathbf{r}_i(0)\Delta\mathbf{r}_j(0)^T\rangle = \delta_{i,j}kT_i\tilde{\mathsf{L}}_i^{-1}, \tag{12.12}$$

where $\Delta\mathbf{r}_i$ is defined by $\Delta\mathbf{r}_i = \mathbf{r}_i - \langle\mathbf{r}_i\rangle$, and the superscript T denotes the transposed matrix. Using Eq. (12.12) one

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[29] Our treatment generalizes a recent paper by Zwanzig (1973) to non-Hamiltonian systems coupled to reservoirs at different temperatures.

[30] This partial integration which amounts to distributing the "deterministic" and "fluctuating" forces in a certain way is not always needed, so that then Eq. (12.3) can be directly inserted into (12.1). Because usually the form of the "deterministic" forces (which are essentially friction forces) can be foreseen, e.g., on physical grounds, one may easily decide in practical cases which way to split up the terms in the equations.

readily derives the following property for the noise sources

$$\langle \mathbf{F}_i(t)\mathbf{F}_j(t')^T\rangle = \delta_{ij}k_BT_i \exp((t-t')\mathsf{L}_i)\tilde{\mathsf{L}}_i^{-1} \tag{12.13}$$

which establishes a relation between the fluctuations (left-hand side) and the dissipation (right-hand side), because the expression

$$\exp((t-t')\mathsf{L}_i)\tilde{\mathsf{L}}_i^{-1} \tag{12.14}$$

just occurs as essential part of the "friction force" in Eq. (12.6) (see also (12.17)). For practical cases it is important to note that in quite a number of applications one may demonstrate that the noise sources are δ-correlated in time.

If our above formalism is specialized to a single reservoir kept at a temperature T, it reduces essentially (with some modifications) to an equation recently derived by Zwanzig (1973). Following Zwanzig we illustrate the above procedure by an example. We consider a single particle with coordinate Q, momentum P, and mass M in the potential $U(Q)$. The systems Hamiltonian is

$$H_s = (P^2/2M) + U(Q). \tag{12.15}$$

The reservoir Hamiltonian is

$$H_b = \sum_j \tfrac{1}{2}p_j^2 + \sum_j \tfrac{1}{2}\omega_j^2(q_j - \gamma_j Q/\omega_i^2)^2. \tag{12.16}$$

We assume linear coupling between S and R. The generalized Langevin equation then reads

$$\begin{aligned} M\,dQ_t/dt &= P_t \\ dP_t/dt &= -U'(Q_t) - \int_0^t dt'\zeta(t')P_{t-t'}/M + F(t). \end{aligned} \tag{12.17}$$

The friction coefficient $\zeta(t)$ is

$$\zeta(t) = \sum (\gamma_j/\omega_j)^2 \cos\omega_j t. \tag{12.18}$$

The fluctuation-dissipation theorem takes the form

$$\langle F(t)\rangle = 0, \qquad \langle F(t)F(t')\rangle = k_BT\zeta(t-t'). \tag{12.18a}$$

By a special choice of frequencies and coupling constants one is led to an equation which is approximately Markovian (compare e.g. R. J. Rubin (1960), Ullersma (1966), G. W. Ford, M. Kac and P. Mazur (1965). We finally note that the above procedure applies equally well if the coordinates $\mathbf{q}$ and $\mathbf{r}$ are quantum mechanical operators. In that case the generalized Langevin equation becomes an operator equation with stochastic operator forces $\mathbf{F}(t)$ which have been e.g., extensively used in laser theory (Haken (1964, 1966, 1970a), Lax (1966c, 1968)).

B. Connection between Langevin equations and Fokker–Planck equations

Langevin equations are contained in Eq. (12.6) as special cases. We want to show that such equations may be equivalent to a Fokker-Planck equation. We assume the Langevin equations in the form

$$\dot{q}_l = k_l(\mathbf{q}) + \sum_{j=1}^{m} g_{lj}(\mathbf{q})\xi_j(t) \qquad l = 1,\cdots,p, \tag{12.19}$$

where q_l are the variables of the system, and k_l and g_{lj} function of $\mathbf{q}$. Here $\xi_j(t)$ are independent Gaussian δ-correlated random functions with

$$\langle \xi_j\rangle = 0, \tag{12.20}$$

$$\langle \xi_l(t+\tau)\xi_j(t)\rangle = \delta_{lj}\delta(\tau). \tag{12.21}$$

One may show that Eq. (12.19) is equivalent to the follow-lowing Fokker–Planck equation [Stratonovich (1963)]:

$$\begin{aligned} \dot{f}(q_1,\cdots,q_m) &= -\sum_{\mu=1}^{m} (\partial/\partial q_\mu)[K_\mu(q_1,\cdots,q_m)\, f(q_1,\cdots,q_m)] \\ &\quad + \tfrac{1}{2}\sum_{\mu,\nu=1}^{m} (\partial^2/\partial q_\mu\,\partial q_\nu)[K_{\mu\nu}(q_1,\cdots,q_m)\, f(q_1,\cdots,q_m)], \end{aligned} \tag{12.22}$$

where the drift and diffusion coefficients are given by

$$K_l(\mathbf{q}) = k_l(\mathbf{q}) + \tfrac{1}{2}\sum_{k,j} (\partial g_{lj}/\partial q_k)\, g_{kj}, \tag{12.23}$$

$$K_{lk}(\mathbf{q}) = \sum_j g_{lj}(\mathbf{q})g_{kj}(\mathbf{q}). \tag{12.24}$$

Obviously, if Eq. (12.19) is given, the drift and diffusion coefficients are fixed by (12.23) and (12.24). However, the inverse is also true. If the drift and diffusion coefficients of the Fokker–Planck equation (12.22) are known one may invert the relations (12.23) and (12.24) in order to find k and g.

Consider the matrix $\mathsf{K} = (K_{lm})$ which is supposed to be symmetric and non-negative definite. (Note that the condition of non-negative definiteness need not hold in systems where the Fokker–Planck equation (12.22) corresponds to a stochastic process connected with a quantum system or to a certain nonequilibrium system). If the above condition, however, holds, according to linear algebra there exists a real, symmetric, nonnegative definite matrix, $G = (g_{lk})$, with $G^2 = K$. Introducing $U = (u_{ij})$ with

$$UKU^{-1} = (K_i{}^0\delta_{ij}), \qquad K_i{}^0 \geq 0, \tag{12.25}$$

we find

$$G = U^{-1}[(K_i{}^0)^{1/2}\delta_{ij}]U, \tag{12.26}$$

and from Eq. (12.23) k_l.

XIII. QUANTUM STATISTICS: THE DENSITY MATRIX EQUATION

In this and the following sections we sketch methods of quantum statistics applicable to quantum systems far from thermal equilibrium. The underlying concept is the same as for classical systems treated in the preceding chapters. The quantum system under consideration is kept far from thermal equilibrium by its coupling to other quantum systems with which it may exchange energy, masses, momentum etc. Thus we are always concerned with the proper system S coupled to reservoir systems denoted by R. Since we are ultimately interested only in the properties of the proper system, we have to devise methods of eliminating the variables or operators of the reservoir system. At present there exist two main elimination techniques, depending on the description of the quantum system $R+S$:

(1) The total system is described by the density matrix equation in the Schrödinger picture. The elimination procedure just mentioned leads to an equation for a *reduced density matrix*, again in the Schrödinger picture.

(2) The total system is described by Heisenberg equations of motion for a suitable set of operators. The elimination procedure leads to *quantum mechanical Langevin equations*.

A. Derivation of a reduced density matrix equation by means of the projector formalism

We describe the elimination technique; following Zwanzig (1964)[31] We denote the density operator of the coupled system $S+R$ by $W(t)$. We decompose the density operator by the identity

$$W(t) = PW(t) + (1-P)W(t), \tag{13.1}$$

where P is a projection operator with

$$P^2 = P. \tag{13.2}$$

Later on we will define P as an operator projecting onto the proper system. (Note that P is not an ordinary operator in the Hilbert space of wave vectors, but acts on the operators in that Hilbert space).

The density matrix equation is written in the form

$$\dot{W}(t) = -iLW(t) = -(i/\hbar)[H, W(t)] \tag{13.3}$$

where L and H are the Liouville operator and Hamiltonian, respectively.[32] Inserting Eq. (13.1) into (13.3) and multiplying (13.3) with P or $(1-P)$, respectively, we obtain the equations

$$P\dot{W} = -iPLPW - iPL(1-P)W, \tag{13.4}$$

$$(1-P)\dot{W} = -i(1-P)LPW - i(1-P)L(1-P)W. \tag{13.5}$$

To eliminate e.g., $(1-P)W$ we integrate Eq. (13.5) obtaining the formal solution

$$(1-P)W(t) = \exp[-i(1-P)Lt](1-P)W(0) - i\int_0^t d\tau \exp[-i(1-P)L\tau](1-P)LPW(t-\tau). \tag{13.6}$$

Inserting Eq. (13.6) into (13.4) we obtain Zwanzig's generalized master equation

$$P\dot{W}(t) = -iPLPW(t) - \int_0^t d\tau PL \exp[-i(1-P)L\tau](1-P)LPW(t-\tau) - iPL\exp[-i(1-P)Lt](1-P)W(0). \tag{13.7}$$

An important problem rests in the choice of the projection operator P, because one has to make later on assumptions (or in other words, certain approximations) whose validity depends on this choice. Zwanzig has defined P such that PW is the diagonal part of $W(t)$ in some specific representation. Following Argyris and Kelley (1964) we may define P as the following trace operation:

$$P = R\,\mathrm{Tr}_R \qquad \text{with} \quad \mathrm{Tr}_R R = 1, \tag{13.8}$$

$$PW(t) = R\,\mathrm{Tr}_R W(t) \equiv R_\rho(t). \tag{13.9}$$

Here R is an operator in the reservoir subspace of the Hilbert space and can be chosen arbitrarily with the constraint of normalization so that P is a projector. Denoting the Liouville operators by indices referring to the proper system S, the reservoir system R, and the interaction between both systems (RS), we decompose L into

$$L = L_S + L_R + L_{RS}. \tag{13.10}$$

Using the abbreviation on the right-hand side of Eq. (13.9), Eq. (13.7) is then transformed into

$$\dot{\rho}(t) = -iL_S\rho(t) - i\,\mathrm{Tr}_R(L_{RS}R\rho(t)) + \int_0^t d\tau Q(\tau)\rho(t-\tau) + I(t) \tag{13.11}$$

with the abbreviations

$$I(t) = -i\,\mathrm{Tr}_R\{L_{RS}\exp[-i(1-P)Lt](1-P)W(0)\}. \tag{13.12}$$

$$Q(\tau) = -\,\mathrm{Tr}_R\{L_{RS}\exp[-i(1-P)L\tau][L_{RS}+L_R]R\}. \tag{13.13}$$

In practical applications one usually expands $Q(\tau)$ into a power series of the interaction operator L_{RS} or a part of it. For more recent examples of applications see e.g., Haake (1969, 1973).

B. Explicit examples of reduced density matrices

The derivation of reduced density matrices in which the operators of the reservoir system have been eliminated up to second order is well known in the literature [Bloch and Wangsness (1953), Argyres (1963), Willis and Bergmann (1962), Weidlich and Haake (1965)]. We therefore present only the main results.

According to Eq. (13.10) we decompose H into

$$H = H_S + H_R + H_{RS}. \tag{13.14}$$

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[31] For a recent review article with applications, see Haake (1973).

[32] One may also treat a more general case, in which L contains also dissipation parts stemming from a preceding elimination procedure.

We put $H_0 = H_S + H_R$ and proceed to the interaction representation

$$\tilde{W} = \exp[(i/\hbar)H_0 t]W\exp[-(i/\hbar)H_0 t], \tag{13.15}$$

$$\tilde{H}_{RS} = \exp[(i/\hbar)H_0 t]H_{RS}\exp[-(i/\hbar)H_0 t]. \tag{13.16}$$

We now assume that $\tilde{H}_{RS}$ has the form

$$\tilde{H}_{RS}(t) = \hbar\sum_k S_k(t)R_k(t), \tag{13.17}$$

with

$$S_k(t) = S_k(0)\cdot\exp(i\Delta\nu_k t), \tag{13.18}$$

where $S_k(t)$, $S_k(0)$ are operators of the proper system S, in the interaction and Schrödinger representations, respectively, whereas R_k are operators of the reservoir system. Explicit examples will be given below. If the reservoirs have a short relaxation time and if the R_k's have no diagonal elements in the energy representation of R, the following *reduced density matrix equation* results:

$$\begin{aligned}\frac{d\tilde{\rho}(t)}{dt} = \sum_{kk'}\{&[S_{k'}(t)\tilde{\rho}(t), S_k(t)]A_{kk'} \\ &+ [S_{k'}(t), \tilde{\rho}(t)S_k]A_{kk'}'\} \equiv L_{\mathrm{red}}\tilde{\rho},\end{aligned} \tag{13.19}$$

where the definition of the reduced Liouville operator is obvious. In Eq. (13.19) $\tilde{\rho}$ is the density matrix of the proper system S in the interaction representation, $[\alpha, \beta] \equiv \alpha\beta - \beta\alpha$, and A, A' are defined as follows:

$$A_{kk'} = \int_0^\infty \exp(-i\Delta\nu_{k'}\tau)\ \mathrm{Tr}_R(R_k(\tau)R_{k'}(0)\rho_R(0))\ d\tau, \tag{13.20}$$

$$A_{kk'}' = \int_0^\infty \exp(-i\Delta\nu_k\tau)\ \mathrm{Tr}_R(R_{k'}(0)R_k(\tau)\rho_R(0))\ d\tau. \tag{13.21}$$

Here $\rho_R(0)$ is the density matrix of the reservoir R at time $t = 0$. In many applications one may assume that $\rho_R(0)$ is a product of canonical distribution functions of reservoirs held at different temperatures T_i. If only a single reservoir with temperature T is present, one may derive the relation

$$\mathrm{Re}A_{k'k} = \mathrm{Re}A_{kk'}\exp(\hbar\Delta\nu_{k'}/k_BT). \tag{13.22}$$

In practice, the coefficients A may often be correlated to experimentally observable damping constants etc. (see below). We now represent two important special cases.

1. The damped harmonic oscillator

Describing the harmonic oscillator (or "Bose field") by the creation and annihilation operators b^+, b, respectively, we may identify

$$H_S = \hbar\omega b^+b,$$

$$S_1(0) = b, \qquad S_2(0) = b^+,$$

$$\Delta\nu_1 = -\omega, \qquad \Delta\nu_2 = \omega,$$

$$R_1 = R_2^+.$$

Further putting $A_{21} = \xi$, $A_{12} = \delta = \xi\exp(-\hbar\omega/kT)$, we find the following density matrix equation[33] [Weidlich and Haake (1965)]

$$d\tilde{\rho}/dt = \delta([b^+\tilde{\rho}, b] + [b^+, \tilde{\rho}b]) + \xi([b\tilde{\rho}, b^+] + [b, \tilde{\rho}b^+]), \tag{13.23}$$

where $b = b(t)$. The physical meaning of δ and ξ becomes obvious by equations for averages defined by

$$\langle 0\rangle = \mathrm{Tr}_S(0\tilde{\rho}). \tag{13.24}$$

$\langle b^+\rangle$ obeys the equation

$$d\langle b^+\rangle dt = -(\xi - \delta)\langle b^+\rangle \tag{13.25}$$

so that $(\xi - \delta)$ can be interpreted as a decay constant, κ, and $\langle b^+b\rangle$ obeys the equation

$$d\langle b^+b\rangle/dt = 2\delta - 2(\xi - \delta)\langle b^+b\rangle. \tag{13.26}$$

Its stationary solution

$$\langle b^+b\rangle = \delta/(\xi - \delta) \tag{13.27}$$

is the mean number $\bar{n}$ of photons in thermal equilibrium with the reservoir, so that $\delta = \kappa\bar{n}$.

2. Arbitrary quantum system described by projection operators P_{ij}

We identify

$$H_S = \sum_j \hbar\nu_j P_{jj}, \tag{13.28}$$

$$S_k(t) = P_{ij}(t), \tag{13.29}$$

$$\Delta\nu_k = \nu_i - \nu_j, \tag{13.30}$$

$$B_k = B_{ij}; \qquad B_{ji} = B_{ij}^+, \tag{13.31}$$

and use $A_{ji,ij}' = A_{ji,ij}^*$. The reduced density matrix equation takes the simple form

$$d\tilde{\rho}(t)/dt = \sum_{ij}\{[P_{ij}\tilde{\rho}, P_{ji}]A_{ji,ij} + [P_{ij}, \tilde{\rho}P_{ji}]A_{ji,ij}^*\}, \tag{13.32}$$

where $P_{ij} = P_{ij}(t)$. To shed light on the meaning of the A's, we represent the equations for $\langle P_{mn}\rangle = \mathrm{Tr}_S(P_{mn}\tilde{\rho})$, following from Eq. (13.32):

$$(d/dt)\langle P_{mn}\rangle = (i\Delta\Omega_{mn} - \gamma_{mn})\langle P_{mn}\rangle, \qquad m \neq n, \tag{13.33}$$

$$(d/dt)\langle P_{mm}\rangle = \sum_j \langle P_{jj}\rangle w_{jm} - \langle P_{mm}\rangle\sum_j w_{mj}, \tag{13.34}$$

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[33] Because the imaginary part of the A's gives rise to mere frequency shifts which can be included in the frequency of the actual oscillator we have kept only the real parts of the A's.

where we have introduced the abbreviations

$$w_{jm} = 2\,\mathrm{Re}A_{jmmj}, \tag{13.35}$$

$$\Delta\Omega_{mn} = -\sum_i \mathrm{Im}(A_{niin} + A_{miim}{}^*), \tag{13.36}$$

$$\gamma_{mn} = \tfrac{1}{2}\sum_i (w_{ni} + w_{mi}). \tag{13.37}$$

Obviously w_{jm} may be interpreted as transition rate from state j to state m.

3. Atom subject to the action of reservoirs

Consider an atom with energy levels i. Denote the creation and annihilation operators of an electron in level i by a_i^+, a_i, respectively. Putting

$$P_{ij} = a_i^+ a_j \tag{13.38}$$

allows us immediately to apply the above formalism to the present case, provided only a single "Leuchtelektron" is treated.

4. Proper system composed of interacting subsystems

The usual procedure is this: One first neglects the interaction (H_{int}) between the subsystem and obtains the reduced density matrix equation of the total system in the form

$$d\rho/dt = \sum_j L_{\mathrm{red},j}\tilde{\rho}, \tag{13.39}$$

where $L_{\mathrm{red},j}$ is the reduced Liouville operator of the subsystem j [compare Eq. (13.19)]. One then adds $(-i/\hbar)[H_{\mathrm{int}}, \tilde{\rho}]$ to Eq. (13.39). This procedure works well if the coupling of the proper system to reservoirs is stronger than within the proper system. The opposite case is still under discussion. In that case, damping terms may be considered as phenomenologically introduced.

XIV. SOLUTIONS OF THE REDUCED DENSITY MATRIX EQUATION

Several methods of solution of the Fokker–Planck equation described in Sec. XI possess direct analogues in the present quantum mechanical case.

A. Time-independent and time-dependent solution of the reduced density matrix equation of a system weakly coupled to reservoirs

We first give a brief outline of our method (Haken (1974b)). We decompose the Liouville operator of the master equation into a part describing the "proper system" and another operator describing the interaction of the proper system with a set of reservoirs. If the proper system is described by a Hamiltonian, the corresponding solutions of the density matrix equation are spanned by M constants of motion and are thus highly degenerate. We demonstrate how this degeneracy is lifted by perturbation theory for degenerate systems and reduce the solution of the original master equation to a much simpler equation of M quantum numbers.

The solution of the master equation of a system described by the Hamiltonian H and weakly coupled to reservoirs, all kept at the same temperature T, is well known:

$$\rho = N\exp(-H/kT).$$

In the following (as elsewhere in this article) we explicitly treat systems *away* from thermal equilibrium.

The reduction procedure. We seek the steady state solution of the master equation

$$\dot{\rho} = L\rho, \tag{14.1}$$

where L is the Liouville operator. More explicitly written Eq. (14.1) reads

$$\dot{\rho} = -(i/\hbar)[H, \rho] + \Lambda_1\rho + \rho\Lambda_2 + \sum_j M_j\rho N_j, \tag{14.2}$$

where H is the Hamiltonian of the proper system and, Λ_1, Λ_2, M_j, N_j are operators which describe the coupling of the proper system to reservoirs. For explicit examples see Sec. III and IV. In the following, we decompose the Liouville operator into two parts

$$L = L_0 + L_1, \tag{14.3}$$

where L_0 contains the Hamiltonian and under certain situations also a part of the operators stemming from the coupling to reservoirs. The unperturbed problem is defined by

$$L_0\rho_0 = 0, \tag{14.4}$$

If

$$\Omega_1, \cdots, \Omega_M \tag{14.5}$$

are operators describing conserved quantities we require also that each polynomial in Eq. (14.5) fulfills (14.4), i.e.,

$$L_0(\Omega_{j_1}{}^{n_1}\cdots\Omega_{j_N}{}^{n_N}) = 0 \tag{14.6}$$

which is e.g., the case for systems described by a Hamiltonian:

$$L_0\rho_0 = -(i/\hbar)[H, \rho_0]. \tag{14.7}$$

In the following we require this general property (14.6). We write the most general solution of (14.4) in the form

$$\rho_0 = f_0(\Omega_1, \cdots, \Omega_M), \tag{14.8}$$

where f_0 is a function still to be determined. We confine our analysis to the case where the Ω's commute[34]: Then the operators (14.5) possess simultaneous eigenfunctions with the corresponding eigenvalues $l_1 \cdots l_M$. These eigenfunctions are denoted by

$$|\, l_1, \cdots, l_M; \alpha\rangle \equiv |\, l; \alpha\rangle. \tag{14.9}$$

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[34] For the general case see Haken (1974b).

α are further quantum numbers which are not specified by the Ω's. Each density matrix, in particular ρ_0, may be written in the form

$$\rho_0 = \sum_{l',\alpha';l,\alpha} | l', \alpha' \rangle \rho_{l',\alpha';l,\alpha} \langle l, \alpha |. \tag{14.10}$$

Multiplying Eq. (14.8) with the eigenfunctions (14.9) and using (14.10) yields immediately

$$\begin{aligned}\rho_{l',\alpha';l,\alpha} &= \langle l', \alpha' | f_0(\Omega_1, \cdots, \Omega_M) | l, \alpha \rangle \\ &= \delta_{\alpha,\alpha'} \delta_{l,l'} f_0(l_1, l_2, \cdots, l_M).\end{aligned} \tag{14.11}$$

In the following we use the abbreviation

$$f_0(l_1, \cdots, l_M) = f_0(l) \tag{14.12}$$

and write correspondingly

$$\rho_0 = \sum_{l,\alpha} | l, \alpha \rangle f_0(l) \langle l, \alpha | \tag{14.13}$$

or, in a shorter way,

$$\rho = \sum_{l} f_0(l) P_l, \tag{14.14}$$

where we define the projection operator P_l by

$$P_l = \sum_{\alpha} | l, \alpha \rangle \langle l, \alpha |. \tag{14.15}$$

In order to determine the function f_0 we form

$$\mathrm{Tr} P_{l'} L_1 \rho_0 = 0. \tag{14.16}$$

This yields for the operator $\Lambda_1 \rho$, which occurs in Eq. (14.2)

$$\begin{aligned}I_1 &\equiv \mathrm{Tr}\Big(\sum_{\alpha'} | l', \alpha' \rangle \langle l', \alpha' | \Lambda_1 \rho\Big) \\ &= \sum_{\alpha'} \langle l', \alpha' | \Lambda_1 \sum_{l,\alpha} f_0(l) | l, \alpha \rangle \langle l, \alpha | l', \alpha' \rangle\end{aligned} \tag{14.17}$$

or, after an evident transformation

$$I_1 = \sum_{l} f_0(l) \sum_{\alpha} \langle l, \alpha | \Lambda_1 | l, \alpha \rangle \delta_{ll'}. \tag{14.18}$$

Correspondingly we find for $\rho \Lambda_2$

$$I_2 = \sum_{l} f_0(l) \sum_{\alpha} \langle l, \alpha | \Lambda_2 | l, \alpha \rangle \delta_{ll'}, \tag{14.19}$$

and for $M_j \rho N_j$

$$I_{3,j} = \sum_{l} f_0(l) \sum_{\alpha,\alpha'} \langle l', \alpha' | M_j | l, \alpha \rangle \langle l, \alpha | N_j | l', \alpha' \rangle. \tag{14.20}$$

Summing up over Eqs. (14.18), (14.19), (14.20) we obtain our fundamental set of equations

$$\sum_{l} K(l', l) f_0(l) = 0, \tag{14.21}$$

with

$$\begin{aligned}K(l', l) = {} & \delta_{l',l} \sum_{\alpha} (\langle l, \alpha | \Lambda_1 | l, \alpha \rangle + \langle l, \alpha | \Lambda_2 | l\alpha \rangle) \\ & + \sum_{\alpha,\alpha',j} \langle l', \alpha' | M_j | l, \alpha \rangle \langle l, \alpha | N_j | l', \alpha' \rangle.\end{aligned} \tag{14.22}$$

We have thus reduced the problem of solving Eq. (14.1) to the solution of Eq. (14.21), where the dimension of "variables" l is now considerably decreased. While, strictly speaking, this reduction scheme applies to the *stationary* solution of the density matrix equation, it may be extended to certain classes of time-dependent problems (compare Sec. XI.C.4).

B. Exact stationary solution of the reduced density matrix for systems in "detailed balance"

The problem is identical (at least in a formal way) with that of Sec. XI.E if we identify $f(\mathbf{m})$ with $\rho_{\mathbf{m}_1,\mathbf{m}_2}$ and substitute $w(\mathbf{m}, \mathbf{n})$ by $w(\mathbf{m}_1, \mathbf{m}_2; \mathbf{n}_1, \mathbf{n}_2)$ in some representation. What is meant here by detailed balance requires a more detailed discussion which goes beyond the scope of the present article. See e.g., Agarwal (1973a), Walls (1974).

C. Exact and approximate relations between moments

The procedure is completely analogous to that of Sec. XI.F, if the q's are replaced by operators, f by the density matrix and L_0, L_1 by the corresponding quantum mechanical operators.

XV. QUANTUM MECHANICAL LANGEVIN EQUATIONS

A. Derivation of generalized Langevin equations

The situation in the quantum mechanical domain is completely analogous to that in the classical described in Sec. XII. We again start from a coupled system $S + R$, which is now described by a Hamiltonian

$$H = H_S + H_R + H_{RS}. \tag{15.1}$$

After having chosen an adequate set of operators s_j and r_l of the systems S and R, respectively, we derive Heisenberg equations by means of the general rule for an arbitrary operator (which does not explicitly depend on time)

$$\dot{\Omega} = (i/\hbar)[H, \Omega]. \tag{15.2}$$

To establish a complete analogy with Sec. XII we assume that H_{RS} is linear in the operators r_l, and that H_R represents (coupled) quantum mechanical oscillators. The equations of motion for $\dot{s}_j$ and $\dot{r}_l$ take a form identical with Eqs. (12.1) and (12.2) (if there $\mathbf{q}$ is replaced by $\mathbf{s}$). The method of solution is also the same as in Sec. XII, provided the correct order of operators is retained. In practical applications so far known to the present author, the partial integration (12.4) need not be performed and Eq. (12.3) may be immediately inserted into (12.1). The structure of the resulting generalized Langevin equation is the same as Eq.

(12.6).[35] However the fluctuating forces are now operators which in general don't commute. In the next section we represent examples of correlation functions of fluctuating forces.

B. Examples for correlation functions of fluctuating forces

1. Bose fields (quantum mechanical harmonic oscillators)

We assume that the equations of motion for the creation and annihilation operators b^+, b contain damping terms of the form $-\kappa b^+$, $-\kappa b$, respectively, i.e., without retardation. The quantum mechanical Langevin equations read [Senitzky (1960, 1961), Lax (1966), see also Haken (1970a)]:

$$\dot{b}^+ = (i\omega - \kappa)b^+ + F^+(t), \tag{15.3}$$

$$\dot{b} = (-i\omega - \kappa)b + F(t). \tag{15.4}$$

If the fluctuating forces F, F^+ (which are operators) are dropped, the solutions of Eqs. (15.3) and (15.4) would obviously violate the commutation relation

$$bb^+ - b^+b = 1.$$

A detailed analysis reveals that this relation is satisfied by the solution of Eqs. (15.3) and (15.4) if the fluctuating forces are taken into account. The correlation functions read

$$\langle F^+(t)\rangle = \langle F(t)\rangle = 0, \tag{15.5}$$

$$\langle F^+(t)F(t')\rangle = 2\kappa\bar{n}(T)\delta(t-t'), \tag{15.6}$$

$$\langle F(t)F^+(t')\rangle = 2\kappa(\bar{n}(T)+1)\delta(t-t'), \tag{15.7}$$

$$\langle F(t)F(t')\rangle = \langle F^+(t)F^+(t')\rangle = 0, \tag{15.8}$$

where $\bar{n}(T)$ is the photon number in thermal equilibrium, provided the oscillator is coupled to a single heat bath at temperature T. If different "modes" λ described by operators b_λ^+, b_λ are coupled to different reservoirs, their fluctuating forces are uncorrelated. It should be noted that the fluctuating forces are not exactly δ-correlated. For a detailed discussion see Lax (1966c) and Kubo (1968).

2. Arbitrary quantum systems described by projection operators P_{ij}

The equations of motion for the operators $P_{ij}(t)$ are assumed in the form[36]

$$\dot{P}_{i_1i_2}(t) = \sum_{j_1j_2} M_{i_1i_2,j_1j_2}P_{j_1j_2}(t) + F_{j_1j_2}(t) \tag{15.9}$$

We decompose M into

$$M = M^{\mathrm{coh}} + M^{\mathrm{incoh}} \tag{15.10}$$

where M^{coh} stems from a Hamiltonian

$$H' = \sum_{mn} c_{mn}P_{mn} \tag{15.11}$$

so that

$$M_{i_1i_2;j_1j_2}{}^{\mathrm{coh}} = (i/\hbar)(c_{j_1i_1}\delta_{j_2i_2} - c_{i_2j_2}\delta_{j_1i_1}). \tag{15.12}$$

The "coefficients" c_{mn} may still be (time-dependent) operators of further quantum systems to which the system described by (15.9) is coupled. M^{incoh} describes all processes which stem from the elimination of the reservoirs. No retardation is assumed. Assuming that the fluctuating forces $F_{ij}(t)$ are δ correlated, their correlation functions are given by

$$\langle F_{i_1i_2}(t)\rangle = 0 \tag{15.13}$$

$$\langle F_{i_1i_2}(t)F_{j_1j_2}(t')\rangle = G_{i_1i_2;j_1j_2}\delta(t-t') \tag{15.14}$$

where

$$G_{i_1i_2;j_1j_2} = \sum_{m,n} \langle\{\delta_{i_2,j_1}M_{i_1j_2;mn} - \delta_{n,j_2}M_{i_1i_2;mj_1} - \delta_{m,i_1}M_{j_1j_2;i_2n}\}\rangle\langle P_{m,n}\rangle. \tag{15.15}$$

It is important to note that in Eq. (15.15) M^{coh} drops out, so that M can be replaced by M^{incoh}.

XVI. THE METHOD OF QUANTUM-CLASSICAL CORRESPONDENCE

This method establishes a correspondence between quantum mechanical quantities and classical quantities as shown in Table II.

The quantum-classical correspondence allows us to replace the solution of a density matrix equation by the solution of a classical differential equation and to calculate quantum mechanical correlation functions by pure c-number procedures. We represent the two cases which have been worked out completely in the literature.

TABLE II. Correspondence between quantum mechanical quantities and classical quantitites.

Quantum mechanical quantity	Classical quantity
Density matrix	(Quasi) distribution function
Operator	Variable or/and differentiation
Density matrix equation	Stochastic equation (generalized or ordinary Fokker–Planck equation)
Expectation values (traces)	Expectation values (averages over distribution function)
Time-ordered correlation functions of operators	Correlation functions of classical quantities

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[35] Generalized Langevin equations for open systems have been recently derived by Kawasaki (1973a, 1973b) along somewhat different lines using Mori's treatment (Mori, 1965).

[36] Our treatment generalizes the result obtained by Haken and Weidlich (1966), see also Haken (1970a), who treated the case $P_{ij} = a_i^+a_j$ where a_i^+ and a_j are creation and annihilation operators of an electron in a one-electron system, and who used the principle of quantum mechanical consistency. The same special case was treated by Lax (1966a), using generalized Einstein relations.

A. Bose operators (quantum mechanical harmonic oscillator)

1. Definition of distribution functions

This case has been extensively treated in the literature [Wigner (1932), Glauber (1963a,b, 1964), Sudarshan (1963), Lax and Louisell (1967), and others]. There are different possibilities of establishing a one-to-one correspondence between the operators b, b^+ and the classical variables u, u^*:

$$b \leftrightarrow u$$

$$b^+ \leftrightarrow u^*$$

(a) *Wigner distribution function*

$$W(u,u^*) = (1/\pi^2)\int\int \exp(-i\beta u - i\beta^* u^*) \times \mathrm{Tr}[\exp(i\beta b + i\beta^* b^+)\rho)\, d^2\beta \tag{16.1}$$

where

$$d^2\beta = d(\mathrm{Re}\beta)\, d(\mathrm{Im}\beta).$$

(b) *Glauber-Sudarshan P-representation*

$$P(u,u^*) = \pi^{-2}\int\int \exp(-i\beta u - i\beta^* u^*) \times \mathrm{Tr}[\exp(i\beta^* b^+)\exp(i\beta b)\rho)]\, d^2\beta. \tag{16.2}$$

(c) *Q representation*

$$Q(u,u^*) = \pi^{-2}\int\int \exp(-i\beta u - i\beta^* u^*) \times \mathrm{Tr}(\exp(i\beta b)\exp(i\beta^* b^+)\rho)\, d^2\beta. \tag{16.3}$$

All definitions correspond to the definition of the distribution function in probability theory of classical variables where b^+ and b would be random functions and e.g. $\mathrm{Tr}[\exp(i(\beta b + \beta^* b^+))\rho] = \chi_W$ would just be the characteristic function. The difference between Eqs. (16.1), (16.2) and (16.3) is due to the prescription of the *order* of the *operators* b^+, b under the trace. Still more general "mappings" are possible, but will not be discussed here.

The relations between W, P, Q are

$$Q(u,u^*) = (2/\pi)\int\int \exp(-2\,|\,u-\alpha\,|^2)W(\alpha,\alpha^*)\, d^2\alpha,$$

$$W(u,u^*) = (2/\pi)\int\int \exp(-2\,|\,u-\alpha\,|^2)P(\alpha,\alpha^*)\, d^2\alpha,$$

$$Q(u,u^*) = (1/\pi)\int\int \exp(-\,|\,u-\alpha\,|^2)P(\alpha,\alpha^*)\, d^2\alpha.$$

2. Calculation of expectation values by means of the distribution functions

In quantum mechanics one is interested in expectation values like

$$\langle g(b,b^+)\rangle = \mathrm{Tr}(g(b,b^+)\rho).$$

The advantage of using the distribution functions is to obtain these expectation values by simple integrations:

$$\mathrm{Tr}(g_N(b,b^+)\rho) = \int\int g_N(u,u^*)P(u,u^*)\, d^2u,$$

$$\mathrm{Tr}(g_A(b,b^+)\rho) = \int\int g_A(u,u^*)Q(u,u^*)\, d^2u. \tag{16.4}$$

In Eq. (16.4) g_N and g_A means that $g(b,b^+)$ has to be arranged by use of the commutation relation $bb^+ - b^+b = 1$ in such a manner that $g_N(g_A)$ is in normal (antinormal) order. To prove Eq. (16.4) we assume that $g_N(g_A)$ can be expanded in a Taylor series. Therefore we have to prove the relations only for

$$\mathrm{Tr}((b^+)^n b^m \rho) = \int\int (u^*)^n u^m P(u,u^*)\, d^2u$$

$$\mathrm{Tr}(b^n (b^+)^m \rho) = \int\int u^n u^{*m} Q(u,u^*)\, d^2u. \tag{16.5}$$

The proof of Eq. (16.5) follows from the fact that the integration of P and Q in (16.5) corresponds to a differentiation of the Fourier transforms, i.e., of χ_P and χ_Q

$$\iint (u^*)^n u^m P(u,u^*)\, d^2u = \left(\frac{\partial}{\partial i\beta^*}\right)^n \left(\frac{\partial}{\partial i\beta}\right)^m \chi_P(\beta,\beta^*)\,|_{\beta=\beta^*=0},$$

$$\iint u^n (u^*)^m Q(u,u^*)\, d^2u = \left(\frac{\partial}{\partial i\beta}\right)^n \left(\frac{\partial}{\partial i\beta^*}\right)^m \chi_Q(\beta,\beta^*)\,|_{\beta=\beta^*=0}.$$

3. Replacement of density matrix equation by generalized Fokker-Planck equation

The density matrix equation

$$\dot{\rho} = L(b^+,b)\rho \tag{16.6}$$

can be replaced by a (generalized) Fokker–Planck equation using the following prescription: (we give as an example the P representation)

$$\rho \longrightarrow P(u,u^*),$$

$$b^+\rho \longrightarrow [u^* - (\partial/\partial u)]P,$$

$$b\rho \longrightarrow uP,$$

$$\rho b \longrightarrow [u - (\partial/\partial u^*)]P,$$

$$\rho b^+ \longrightarrow u^* P.$$

For products of operators the correspondence is established by induction yielding

$$\Omega \equiv \Omega_1(b^+,b)\rho\Omega_2(b^+,b) \equiv \Omega_1(u^* - \partial/\partial u, u)\Omega_2(u^*, u - \partial/\partial u^*)P.$$

B. Arbitrary quantum systems described by projection operators

1. Definition of distribution function for expectation values

Again, as in XVI.A.1, different definitions are possible, depending on the sequence of operators. Here we define f

by Haken (1969b)[37]

$$f(v) = N\int \exp(-\sum_{ik} v_i\ \kappa_{ik}) \times \mathrm{Tr}(\prod_{ik} \exp(\kappa_{ik}P_{ik})\rho)\ d\{\kappa\} \tag{16.7}$$

where N is the normalization constant, and κ_{ik} are classical complex quantities, with

$$\kappa_{ik} = -\kappa_{ki}^{*}.$$

The v_{ik}'s are classical variables which are associated with each projection operator:

$$v_{ik} \leftrightarrow P_{ik}; \qquad v_{ik} = v_{ki}^{*}.$$

We order the operators in the following way

$$O = O_L O_M O_R = \prod_{ik} \exp(\kappa_{ik}P_{ik}), \tag{16.8}$$

where

$$O_L = (1, 2)(1, 3)(1, 4)\cdots(1, n)(2, 3)(2, 4)\cdots \cdots(2, n)\cdots(n-2, n-1)(n-2, n)(n-1, n) \quad , \tag{16.9}$$

$$O_M = (1, 1)(2, 2)\cdots(n, n), \tag{16.10}$$

$$O_R = (n, n-1)(n, n-2)(n-1, n-2)\cdots \cdots(n, 2)(n-1, 2)\cdots(3, 2)(n, 1)\cdots(3, 1)(2, 1). \tag{16.11}$$

We have used the following definitions

$$i < k,$$

$$\kappa_{ik} = \xi_{ik},$$

$$(i, k) = \exp(\xi_{ik}P_{ik}) = (1 + \xi_{ik}P_{ik}) \tag{16.12}$$

$$i = k$$

$$\kappa_{ii} = \xi_{ii} = \eta_i,$$

$$(i, i) = \exp(\xi_{ii}P_{ii}) \equiv \exp(\eta_i P_{ii}) = 1 + [\exp(\eta_i) - 1]P_{ii} \tag{16.13}$$

$$i > k,$$

$$\kappa_{ik} = \tilde{\xi}_{ik},$$

$$(i, k) = \exp(\tilde{\xi}_{ik}P_{ik}) = (1 + \tilde{\xi}_{ik}P_{ik}). \tag{16.14}$$

The *expectation value* of P_{lm} is given by

$$\mathrm{Tr}(P_{lm}\rho) = \int\cdots\int v_{lm} f(v)\ d\{v\}, \tag{16.15}$$

where the integration runs over all variables $v_{ik}(=v_{ki}^{*})$ over the whole complex plane.

If $\rho(t)$ obeys the usual density matrix equation (13.19) (which is of first order in its time derivative, the heat baths being Markovian) it is possible to calculate multitime averages of the form

$$\mathrm{Tr}(P_{i_1k_1}(t_1)P_{i_2k_2}(t_2)\cdots P_{i_nk_n}(t_n)\rho(t_0)), \tag{16.16}$$

with

$$t_1 > t_2 > \cdots > t_n,$$

by means of a single-time distribution function.

2. Replacement of density matrix equation by generalized Fokker-Planck equation

The density matrix equation

$$\rho(t) = \rho(t_0) + \int_{t_0}^{t} K^{(0)}(t, \tau)\rho(\tau)\ d\tau + \int_{t_0}^{t} d\tau\{ \sum_{iki'k'} K_{ikk'i'}(t, \tau)P_{ik}\rho(\tau)P_{k'i'} + \sum_{ik} K_{ik}^{(1)}(t, \tau)P_{ik}\rho(\tau) + \sum_{ik} K_{ik}^{(2)}(t, \tau)\rho(\tau)P_{ik}\} \tag{16.17}$$

can be replaced by the generalized Fokker–Planck equation [Haken (1969b)]

$$f(t) = f(t_0) + \int_{t_0}^{t} K^{(0)}(t, \tau)\, f(\tau)\ d\tau + \int_{t_0}^{t} d\tau\left\{ \sum_{iki'k'} K_{ikk'i'}(t, \tau) \sum_{\lambda\mu} M_{k'i',ik;\lambda,\mu}\left(\frac{\partial}{\partial v}\right) v_{\lambda\mu} + \sum_{ik} K_{ik}^{(1)}(t, \tau) \sum_{\lambda\mu} N_{ik\lambda\mu}^{(1)}\left(\frac{\partial}{\partial v}\right) v_{\lambda\mu} + \sum_{ik} K_{ik}^{(2)}(t, \tau) \sum_{\lambda\mu} N_{ik\lambda\mu}^{(2)}\left(\frac{\partial}{\partial v}\right) v_{\lambda\mu}\right\} f(\tau). \tag{16.18}$$

This equation is to be supplemented by the constraint $\sum v_{ii} = 1$. Using the rule

$$\kappa_{ik} \to -(\partial/\partial v_{ik}), \tag{16.19}$$

we define the quantities M, $N^{(1)}$, $N^{(2)}$ as follows:

$$M_{ik,k'i',\lambda\mu} = \sum_{mnl} A_{ikmn}B_{k'i'nl}\tilde{C}_{ml\lambda\mu} \exp(\kappa_{nn} - \kappa_{ll}), \tag{16.20}$$

where

$$A_{ikmn} = \delta_{im}O_L^{k\to n} - \kappa_{mi}\delta_{m<i}O_L^{k\to n}, \tag{16.21}$$

$$B_{ikmn} = \delta_{kn}O_R^{m\leftarrow i} - \kappa_{kn}\delta_{n<k}O_R^{m\leftarrow i}, \tag{16.22}$$

---

[37] This type of distribution function had been introduced by Haken, Risken, and Weidlich, Z. Phys. **206**, 355 (1967), where instead of P_{ik} we had used $a_i^{+}a_k$. a_i^{+} and a_k are the usual creation and annihilation operators of Fermions. In the one-particle subspace, $a_i^{+}a_k$ just obeys the relation of projection operators $P_{ij}P_{kl} = \delta_{jk}P_{il}$. The definition (16.7) secures that f is a real function (which is not always positive, however). Equation (16.7) allows for a number of modifications and extensions.

and $\delta_{m<i} = 1$ for $m < i$, and $=0$ otherwise. Here

$$O_L^{m\to k} = \delta_{mk} + \sum \kappa_{ml_1}\kappa_{l_1l_2}\cdots\kappa_{l_jk}$$

and the summation runs over all ways from m to k with

$$\begin{aligned} &m < l_1 < l_2 \cdots < k && \text{for } k \geq m, \\ &O_L^{m\to k} = O && \text{for } m > k, \end{aligned} \tag{16.23}$$

Then

$$O_R^{m\leftarrow l} = \delta_{ml} + \sum \kappa_{ml_j}\cdots\kappa_{l_2l_1}\kappa_{l_1l}$$

and the sum runs over all ways from l to m with

$$\begin{aligned} &m > l_i > l_{i-1}\cdots > l_2 > l_1 > l && \text{for } m \geq l, \\ &O_R^{m\leftarrow l} = O && \text{for } m < l, \end{aligned} \tag{16.24}$$

$$\tilde{C}_{ik,lm} = \begin{cases} C_{iklm} = \delta_{il}(\delta_{km} - \delta_{k<m}\kappa_{km}), & \left\{\begin{array}{l} i < k, \\ l < m, \end{array}\right. \\ D_{ii,lm} = \delta_{il}\delta_{im}, & \left\{\begin{array}{l} i \equiv k, \\ l \leq m, \end{array}\right. \\ E_{ik,lm} = \delta_{km}(\delta_{il} - \kappa_{li}\delta_{i<l}) \exp(-\kappa_{ii} + \kappa_{kk}), & \left\{\begin{array}{l} i > k, \\ l > m, \end{array}\right. \end{cases} \tag{16.25}$$

$$\tilde{C}_{ik,lm} = O, \qquad \text{otherwise},$$

$$N_{ikmn}^{(1)} = \begin{cases} \left.\begin{array}{ll} H_{ik,mm} = \delta_{im}(\delta_{km} - \kappa_{km}\delta_{m<k}), & \\ H_{ik,mn} = \delta_{im}(\delta_{kn} - \kappa_{kn}\delta_{n<k}) + \kappa_{mn}\delta_{n<m}\delta_{in}(\delta_{kn} - \kappa_{kn}\delta_{n<k}), & m > n \end{array}\right\}, & i \geq k, \\ \sum\limits_{m'n'} B_{ikm'n'} \exp(\kappa_{m'm'} - \kappa_{n'n'})\tilde{C}_{m'n'mn}, & i < k, \end{cases} \tag{16.26}$$

$$N_{ikmn}^{(1)} = O \qquad \text{for} \quad i \geq k,\, m < n,$$

$$N_{iklm}^{(2)} = \begin{cases} \left.\begin{array}{ll} F_{ik,ll} = \delta_{il}\delta_{kl} - \kappa_{li}\delta_{l<i}\delta_{kl}, & \\ F_{ik,lm} = \delta_{km}(\delta_{li} - \kappa_{li}\delta_{l<i}) + \delta_{kl}\kappa_{lm}\delta_{l<m}(\delta_{il} - \kappa_{li}\delta_{l<i}), & l < m \end{array}\right\}, & i \leq k, \\ \sum\limits_{m'n'} A_{ikm'n'}\tilde{C}_{m'n'lm}, & i > k, \end{cases} \tag{16.27}$$

$$N_{ikmn}^{(2)} = O \qquad \text{for } i \leq k,\, l > m.$$

Because the operator acting on f on the right-hand side of Eq. (16.18) is *linear* in $v_{\lambda\mu}$, the Fourier transform of f obeys a partial differential equation which is of only first order in its derivatives. Thus the solution of this equation may offer certain advantages over the direct solution of Eq. (16.18).

3. Projection onto macroscopic variables

Our Eq. (16.18) applies to a single atom with two energy levels, or a spin 1/2, to multi-level atoms, as well as to a complicated many-body problem. For a discussion of its solutions, it is thus certainly necessary to treat specific examples.[38] On the other hand, under certain circumstances it is possible to perform strong simplifications even in rather general cases. Indeed, in many cases of practical importance, the system under consideration consists of many equivalent subsystems. Examples are spins in external fields, or laser-atoms interacting with the light field. In these examples the individual subsystems interact with the external fields in a similar way, i.e., by their total (macroscopic) electric or magnetic moments (after certain phase factors have been transformed away, see e.g., Sec. III). In these cases, it is advantageous first to introduce projection operators for each subsystem: $P_{ik,\mu}$ and to formulate the density matrix equation by means of these $P_{ik,\mu}$. It reads

$$\rho(t) = L\rho(\tau), \tag{16.28}$$

where L is a linear operator [see Eq. (16.18)]. In our present case, L consists of a sum over the subsystems:

$$L = \sum_\mu \tilde{L}_\mu(P_{ik,\mu}) \equiv \sum_\mu \tilde{L}(P_{ik,\mu}), \tag{16.29}$$

where the latter equation expresses the fact that the subsystems are equivalent. We now introduce macroscopic variables:

$$V_{ik} = \sum_\mu v_{ik\mu} \tag{16.30}$$

---

[38] For example, in the case of a two-level atom, f if built up of δ-functions (W. Weidlich, private communication).

and define

$$f(t) = \int d\{\kappa\} \exp\{-\sum_{ik} \kappa_{ik} V_{ik}\} \, tr((\prod_{\nu} O_{\nu})\rho), \tag{16.31}$$

where

$$O_{\nu} = \prod_{ik} \exp(\kappa_{ik} P_{ik,\nu}). \tag{16.32}$$

Because the O_{ν}'s commute, we may decompose

$$\prod_{\nu} O_{\nu} = \prod_{\nu}{}^{(\mu)} O_{\nu} \cdot O_{\mu},$$

where (μ) indicates, that the factor $\nu = \mu$ is to be omitted. We multiply Eq. (16.28) from the left by O and take the trace with respect to the whole system:

$$\begin{aligned} \mathrm{Tr}(O\rho) &= \mathrm{Tr}(OL\rho(\tau)) = \sum_{\mu} tr(O\tilde{L}(P_{ik,\mu})\rho) \\ &= \sum_{\mu} \mathrm{Tr}^{(\mu)}[(\prod_{\nu}{}^{(\mu)} O_{\nu}) \, \mathrm{Tr}_{\mu}(O_{\mu}\tilde{L}(P_{ik,\mu})\rho)]. \end{aligned} \tag{16.33}$$

It had been shown (Haken 1969b, 1970a) that

$$\mathrm{Tr}_{\mu}(O_{\mu}\tilde{L}(P_{ik,\mu})\rho) = h(\kappa_{ik}, \partial/\partial\kappa_{ik}) \, \mathrm{Tr}_{\mu}(O_{\mu}\rho). \tag{16.34}$$

Note that O_{μ} is a function of κ_{ik} due to Eq. (16.32). The right-hand side of Eq. (16.33) can thus be written in the form

$$(16.33) = \sum_{\mu} \mathrm{Tr}^{(\mu)}[(\prod_{\nu}{}^{(\mu)} O_{\nu}) h(\kappa_{ik}, \partial/\partial\kappa_{ik}) \, \mathrm{Tr}(O_{\mu}\rho)] \tag{16.35}$$

$$= \sum_{\mu} \mathrm{Tr}[\prod_{\nu}{}^{(\mu)} O_{\nu} \cdot h(\kappa_{ik}, \partial/\partial\kappa_{ik}) O_{\mu}\rho]. \tag{16.36}$$

Note that we can always use the cyclic properties of the traces, if needed.

Now let us make use of the fact that h is of first order in the derivatives $\partial/\partial\kappa_{ik}$ [compare Eq. (16.18)]. According to Leibniz's rule of differentiating products, we immediately find

$$\mathrm{Tr}(O\rho) = h(\kappa_{ik}, \partial/\partial\kappa_{ik}) \mathrm{Tr}(\prod_{\nu} O_{\nu}\rho). \tag{16.37}$$

We multiply Eq. (16.37) with

$$\exp(-\sum_{ik} \kappa_{ik} V_{ik})$$

and integrate over κ_{ik}. This leaves us with

$$f(V_{ik}, t) = \chi(V_{ik}, \partial/\partial V_{ik}) f(V_{ik}, \tau), \tag{16.38}$$

where χ is a linear operator defined on the right-hand side of Eq. (16.18), if the small v_{ik}'s are replaced by the big ones, V_{ik}'s. A simple analysis shows that the condition $\sum_i v_{ii} = 1$ is now to be replaced by $\sum V_{ii} = N$, where N is the number of subsystems. The importance of the result (16.38) is the following rule: while $f(v_{ik}, t)$ of a single subsystem may show wild fluctuations (e.g., it consists of δ functions), the macroscopic variables V_{ik} possess a smooth distribution, which changes but little. Thus in many cases of interest it can be shown that we may neglect derivatives of e.g., higher than second order, so that Eq. (16.38) then actually reduces to an ordinary Fokker–Planck equation.

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