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STUDIES IN STATISTICAL DYNAMICS

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CONTENTS

Synopsis

It is attempted to give a comprehensive theoretical account of the dynamics of statistical phenomena in physics. On the basis of merely a few simple constraints one arrives at equations of motion for a field, which field may be of type of a probability density. The basic equations of motion are linear integro-differential equations. In § 3 we discuss the formal properties of solutions of the equations of motion. Next, in § 4 we derive the family of degradation functions—entropy being one example—which account for common properties of systems and for the approach towards equilibrium. In § 5 we treat the question of differential equations of motion. We find a remarkable limitation of differential equations. Finally, § 6 contains a number of exact solutions of simple integral equations with divergent kernels.

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§ 1. Introduction

In the following we shall study the general theoretical framework for dynamical phenomena in statistical physics. We aim to discuss, on an abstract basis, the behaviour in time of physical systems. If a system is described by a time-dependent field within a generalized space, one can single out a few properties which must be common to many, or to all, phenomena in statistical physics. These properties can be reformulated as a framework for equations of motion of the field, in terms of integral equations or integro-differential equations. Within this framework we derive a number of consequences as to the possible behaviour of the field, which results are obtained even before definite equations of motion are stipulated.

During our studies, the topic gradually separated into four distinct, though not unconnected, parts. One part is the question of linear equations of motion, and their formal properties. Another concerns actual analytic solutions of simple cases. A third question is that of common properties of systems, accounted for by a family of degradation functions, of which entropy is merely one example. The fourth part concerns differential equations, both as approximations and on their own. They turn out to have a surprising limitation. As it will appear, our account of each subject is incomplete, but we hope that it is carried far enough to elucidate the main questions in each instance.

As indicated, we enter on questions familiar from widely different fields of research. It may well be that many of the results at which we arrive are discussed with greater precision and in more detail in texts dealing with mathematical probability theory, with statistical mechanics, or with wave mechanics. Our aim is merely to build up a simple, consistent framework. We try in particular to avoid concepts and structures, however admirable, that are unnecessary for our purpose. The reader is therefore asked to take much the same detached attitude as Gibbs in his discussion of statistical

mechanics, and to consider primarily whether there is agreement between the elementary premises and the conclusions.

Though abstract, these studies were in part prompted by a practical necessity. It arose in our previous investigations of a minor subgroup of phenomena, i.e. the integral equations occurring in atomic collisions where a penetrating particle dissipates energy and exchanges momentum in a substance[12, 13]. Characteristic cases are here, firstly, the multiple scattering in angle of the incoming particle by a randomly distributed substance[3, 18]; secondly, the distribution in energy of an incoming particle, as a function of time, this being a one-way process with only decrease of energy; thirdly, the quite complicated phenomena of changes of transverse energy in directional effects for fast charged particles moving through crystals[14]. We have worked out a number of analytic solutions of the first two cases, with divergent total cross sections (cf. § 6). For directional effects there is a particular need of establishing the rules to be followed when introducing approximation procedures – like differential equations or perturbation theory – in attempts to solve the equations of motion.

Another group of phenomena may be exemplified by the dynamics of a degenerate free electron gas where, by means of the dielectric description, one can study linear dynamic properties in considerable detail and follow the trend towards equilibrium.

It can be useful for the reader to take cases of the above kind as possible illustrations in the following. We might mention that although the problem of the behaviour in time and in phase space of an ensemble is within the scope of the present discussion, the reader should hardly, in the beginning at least, consider the phase space ensemble as a representative example (cf. § 5).

§ 2. Basic Properties of Systems

This chapter should serve two purposes. As a secondary purpose we introduce the terminology and concepts to be used in the following. Primarily, however, we want to specify basic physical properties which characterize various types of systems. The properties are introduced as six constraints, of which four are common to those systems that are of main interest in this paper. Other constraints specify systems we wish to study first, because of their simple basic properties or because they are of interest in applications. The results derived in the following chapters rely on a varying number of constraints, to be specified in each case.

The Basic Constraints

We suppose that phenomena in statistical physics, e.g. of the kind mentioned above, can be described by a function, $a(x,t)$, depending on a spatial variable x, within a generalized space, and on a time variable, t. The state of a system is completely specified at a time t if $a(x,t)$ is given for all x. The physical quantities that can be calculated within such systems will be discussed later.

The space variable x is usually considered as a continuum variable in a space of one or several dimensions. When necessary, we write the space variable explicitly as a vector, $\vec{x}$. It may also be a discrete variable $k = 1, 2, 3, \ldots N$, with N finite or infinite. The discussion is usually formulated for continuum variables and is meant to include the discrete case.

We now introduce a number of constraints, specifying properties of the systems in question. The first constraint, supposed to be valid for all systems, is that the state of a system at a given time uniquely determines its state at any later time, or

$$a(x,t) \text{ given for all } x \rightarrow a(x',t') \text{ for all } x' \text{ and all } t' > t. \quad (2.1)$$

We have introduced the variable t as a familiar time concept. The variable t may, however, also represent other quantities with similar one-way properties, e.g. in atomic collisions the path length moved by a particle, or even the energy of a particle during slowing-down.

The second constraint corresponds to conservation of probability in simple phenomena. We demand that

$$\int \dot{a}(x,t)\,dx = 0, \quad (2.2)$$

where $\dot{a}(x,t) \equiv \frac{\partial}{\partial t} a(x,t)$. According to (2.2) we may usually suppose that $\int a(x,t)\,dx = \text{const.}$ and can be normalized to unity, which will be a standard convention. Still, it occasionally becomes convenient to treat functions which can not be normalized, even though (2.2) applies.

The third constraint indicates that the field $a(x,t)$ is not unlike a probability density. We assume that $a(x,t)$ is real and non-negative,

$$a(x,t) \text{ real}, \qquad a(x,t) \geq 0. \quad (2.3)$$

This constraint turns out to have remarkable consequences.

The fourth constraint imposes superposition, thereby confining the phenomena to a linear behaviour. We demand that if $a_1(x,t)$ and $a_2(x,t)$ are

solutions of the equations of motion, then also $\lambda_1 a_1(x,t) + \lambda_2 a_2(x,t)$ will be a solution, or

$$a_1(x,t) \text{ and } a_2(x,t) \rightarrow \lambda_1 a_1(x,t) + \lambda_2 a_2(x,t). \tag{2.4}$$

To be more precise, and in view of the other constraints, the content of eq. (2.4) is: If a_1 and a_2 are solutions for $t \geq t_0$, and if $\lambda_1 a_1(x,t_0) + \lambda_2 a_2(x,t_0)$ is an allowed function, then $\lambda_1 a_1(x,t) + \lambda_2 a_2(x,t)$, $t \geq t_0$, is a solution.

The constraint (2.4) might seem to be a serious limitation of the scope of the treatment. It does, however, correspond to the basic cases one must necessarily treat at first. Moreover, it should be remembered that in the quite general cases of quantum theory or of dynamics of ensembles one is in fact concerned with linear equations of motion.

We next come to a useful limitation in many initial studies. In mechanics, for instance, it is often profitable to study first the case of a time-independent Hamiltonian. One may then later, at least to some extent, study a time-dependent Hamiltonian, e.g. in order to initiate and terminate the phenomenon in question. The fifth constraint limits the treatment to time-independent dynamics, or invariance of solutions towards displacement in time,

$$a(x,t) \rightarrow a(x,t+\tau), \text{ any fixed real } \tau. \tag{2.5}$$

For practical purposes one further simplification is often valid. The sixth constraint concerns invariance of solutions towards displacement in space, or

$$a(x,t) \rightarrow a(x+\xi,t), \text{ for any real } \xi. \tag{2.6}$$

The displacement may be within a multi-dimensional space $\vec{x}$.

Equations of Motion

We construct next the equations of motion, as they emerge by successive introduction of the constraints. We always assume validity of the first constraint, (2.1). Although it is possible to consider non-linear cases, we shall for the present disregard them, and apply the fourth constraint, (2.4). From the first and fourth constraints we therefore conclude that if the field $a(x',t')$ is known at time t' then

$$a(x,t) = \int dx' T(x,t;x',t') a(x',t'), \quad t > t', \tag{2.7}$$

or

$$a_k(t) = \sum_j T_{kj}(t,t') a_j(t'), \quad \bar{a}(t) = \bar{\bar{T}}(t,t') \bar{a}(t').$$

The quantity T will be called the propagator, having the property

$$T(x,t;x',t) = \delta(x-x'). \tag{2.8}$$

This way of stating the constraint is, however, somewhat indefinite at first, although it will be useful later. When we ask for the equations of motion, it is more profitable to summarize the first and fourth constraints as an expression for the time derivative of $a(x,t)$, which must receive a contribution from the point y, of type of $\Gamma(x,y,t)a(y,t)$, so that

$$\dot{a}(x,t) = \int dy \Gamma(x,y,t) a(y,t), \tag{2.9}$$

where the unspecified integral, as always, extends over the total system and may be multi-dimensional. Next, we apply the second constraint, (2.2), demanding conservation. It implies that, in (2.9), we must have

$$\int dx \Gamma(x,y,t) = 0, \quad \text{for all } y, \tag{2.10}$$

for if (2.10) did not hold, one could choose such functions $a(y,t)$ in (2.9), e.g. δ-functions, as would violate eq. (2.2).

We may make a preliminary reformulation of (2.10). Outside the diagonal, i.e. for $x \neq y$, we alternatively denote $\Gamma(x,y,t)$ as $G(x,y,t)$. The equation (2.10) is then formally fulfilled for any $G(x,y,t)$ if Γ in (2.9) is given by

$$\Gamma(x,y,t) = G(x,y,t) - \delta(x-y)\int dx' G(x',x,t). \tag{2.11}$$

The third constraint, (2.3), demands that $a(x,t)$ remains real and non-negative. Suppose that, in some point x_0, $a(x_0,t) = 0$, whereas in other points $a(x,t)$ is arbitrary but non-negative. In the equation of motion, (2.9), we must then demand $\dot{a}(x_0,t) \geq 0$. But this requires that $\Gamma(x,y,t)$ is non-negative for $x \neq y$, or

$$G(x,y,t) \text{ real}, \qquad G(x,y,t) \geq 0. \tag{2.12}$$

The total result of the four constraints can now be written as a basic integral equation, superseding the preliminary equations (2.11) and (2.12)

$$\dot{a}(x,t) = \int dy \{G(x,y,t)a(y,t) - G(y,x,t)a(x,t)\}, \quad G(x,y,t) \geq 0. \tag{2.13}$$

This equation is the starting-point of most of our further studies.

As to the behaviour of $G(x,y)$, we generally consider it as a continuous function, but it may diverge for $y \to x$. In fact, we allow that $\int_{|x-y|>\varepsilon} dy G(y,x) \to \infty$ for $\varepsilon \to 0$. The permitted degree of divergence de-

pends on the symmetry of the system, as mentioned in § 6. The limit of $G(x,y)$, or part of it, becoming infinitely narrow is discussed in connection with differential equation approximations in § 5.

In the majority of the cases to be studied here, we add the fifth constraint, (2.5), so that solutions are invariant towards time displacements. It follows from eq. (2.13) that then $G(x,y,t+\tau) = G(x,y,t)$, for all τ, and eq. (2.13) reduces to

$$\dot{a}(x,t) = \int dy\{G(x,y)a(y,t) - G(y,x)a(x,t)\}, \quad G(x,y) \geq 0. \tag{2.14}$$

Finally, we occasionally invoke the special constraint (2.6), concerning displacement in space, according to which, apparently, in e.g. (2.14)

$$G(x,y) = G(x-y). \tag{2.15}$$

Classification of Systems

Consider time-independent systems, so that eq. (2.14) is valid. We have shown that $G(x,y) \geq 0$, but in regions of considerable size one can then have that $G(x,y) = 0$. This may result in complete lack of connection, both directly and indirectly, between some regions of x-space. Such systems must be regarded as divisible into subsystems. We therefore define an elementary unit, the indivisible system. To this end, consider two points, x_1 and x_2, within a system. Let first $a(x,t_0) = \delta(x-x_1)$, and if then the integral equation implies that $a(x_2,t) \neq 0$ at some later time $t > t_0$, then x_1 is said to communicate with x_2. This communication is called direct if it occurs in one step, i.e. if $G(x_2,x_1) \neq 0$.

A system is now called indivisible if, for any set of points (x_1,x_2) within it, both x_1 communicates with x_2, and x_2 with x_1. The system is indivisible, with direct communication, if $G(x_1,x_2) \neq 0$ for all x_1,x_2 within it. In the following, we are mainly concerned with indivisible systems. Some characteristic examples are discussed in the beginning of § 3.

An opposite extreme to an indivisible system is, as indicated above, a system which can be divided into completely unconnected subsystems. This will be called a separable system.

In between these two extremes there is a considerable range of systems with partial communication of varying type. Of these systems we shall only be interested in one-way systems. They are essentially one-dimensional systems, and may for instance be characterized by the condition that x_1 communicates with x_2 if and only if $x_1 < x_2$.

Projections

The state of the system at the time t is given by the distribution in space, $a(x,t)$, the integral of which is conserved in time. One may then calculate projections (or averages) of various functions. There are two types of projections.

Firstly, for a function $f(x)$, depending on the spatial variable x, the projection is

$$\langle f(x) \rangle = \int f(x) a(x,t) dx, \tag{2.16}$$

and will in general be a function of time. Note that for discrete variables, $f(x) \to f_k$, $a(x,t) \to a_k(t)$, this formula becomes the scalar product of two vectors, $\langle f \rangle = \sum_k f_k \cdot a_k(t) = \bar{f} \cdot \bar{a}(t)$. It is thus the projection of a fixed vector $\bar{f}$ on a time-dependent vector $\bar{a}(t)$. Obviously, the function f may also be allowed to depend explicitly on time, $f = f(x,t)$.

Secondly, instead of (2.16), one may consider projections of another kind of functions, i.e. functions depending on a,

$$\langle q(a) \rangle = \int q(a(x,t)) a(x,t) dx, \tag{2.17}$$

or $\sum_k q(a_k(t)) a_k(t)$ for discrete variables. The functions $q(a)$ may be denoted as spectral functions. It is possible, but less common, to have projections of functions depending on both x and a.

Transformation of Spatial Variables

Suppose that the one-dimensional spatial variable x is replaced by $z = z(x)$, and that $z(x)$ changes monotonically with x, the latter in order to have simple uniqueness of transformation. Since then

$$a(x,t) dx = a(x,t) \frac{dx}{dz} dz,$$

the distribution $a_1(z,t)$ on the z-axis is

$$a_1(z,t) = a(x,t) \left| \frac{dx}{dz} \right|, \tag{2.18}$$

where $|dx/dz|$ becomes the Jacobian in the general multi-dimensional case. In all transformations the quantity

$$dP = a(x,t) dx = a_1(z,t) dz \tag{2.19}$$

remains invariant, as does its integral over space.

Conjugate Field

When the integral equation of motion (2.9) or (2.13) is given for the field $a(x,t)$, there exists immediately one other equation of motion, valid for a different field. In fact, introduce a field $b(x,t)$, obeying the equation*

$$\dot{b}(x,t) = -\int dy b(y,t)\Gamma(y,x,t) = -\int dy\{b(y,t) - b(x,t)\}G(y,x,t), \quad (2.20)$$

or in matrix form $\dot{\bar{b}} = -\bar{b}\,\bar{\bar{\Gamma}}$. This equation of motion, which we call conjugate to (2.9) and (2.13), is governed by the transposed Γ-matrix. We describe the field $b(x,t)$ as conjugate to $a(x,t)$. Note that we introduce a minus sign in the time derivative in (2.20). This is so far a convention. Of the conjugate field we know immediately that it has an equilibrium solution

$$b^0(x) = \text{const.}, \qquad \bar{b}^0 = C\bar{1}, \quad (2.21)$$

as is obvious from (2.20). We can evidently also conclude that, if $b(x,t)$ is non-negative, the function $b(x',t')$ is non-negative at all previous times $t' < t$. In this backward sense, the conjugate field therefore fulfills the third constraint, (2.3). We do not, however, know beforehand whether the conjugate field obeys a conservation law.

It turns out that, in the discussion of solutions of the equation of motion for $a(x,t)$, the conjugate field is often a useful auxiliary quantity.

The Current

For a quantity with conservation in space one can introduce a current when the equation of motion is known. In one dimension this is straightforward. From knowledge of the transition rate $G(x',y)$ between any two points one finds immediately that the total flow per unit time in the positive direction past a point x will be

$$j(x,t) = -\int^x dx' \int_x dy\{G(x',y)a(y,t) - G(y,x')a(x',t)\}, \quad (2.22)$$

where the integration over y alternatively might be allowed to be between the system boundaries. The current then fulfills the equation

$$\dot{a}(x,t) = -\frac{\partial}{\partial x} j(x,t). \quad (2.23)$$

* An equation of motion of type of (2.20) is often called the backward equation, (2.13) being the forward equation.

Boundary Conditions and Sources

In the following we always discuss the behaviour of systems which are isolated. There is then no current away from the system or into it. For discrete systems with finite N this condition is obviously fulfilled by the equations of motion (2.13). For a continuum system defined in a finite closed region, i.e. including its boundaries, the demand of an isolated system is also straightforward. When the system is infinite, however, the boundary conditions are less simple. For practical reasons, we usually consider a finite but arbitrarily large interval, L. The system is then supposed either to have zero current at the boundaries, or to be periodic. The two conditions are quite different, the former imposing a rest system and the latter allowing transformations to moving coordinate systems. These questions are elucidated by an example in § 6.

Note that when we introduce the conjugate field, as well as eigenfunctions of the fields, the prescribed boundary conditions must be obeyed in each instance.

An alternative way of analysing the dynamics of systems is to introduce sources of the field, depending arbitrarily on space and time. One then adds a term $S(x,t)$ on the right-hand side of e.g. (2.14), and finds the forced motion. This procedure is familiar from, for instance, the dielectric description of an electron gas. The method can be advantageous, but we shall not employ it.

§ 3. Properties of Solutions

In this chapter we derive a number of general properties of the solutions of the integral equation. We first obtain the basic result that, for indivisible systems, there is exactly one equilibrium solution, and it is everywhere positive. Next, the equations of motion are transformed to normal coordinates, and the field is found to tend towards the equilibrium. Third, we treat summarily the general question of eigenvalues and eigenfunctions of the field and of the conjugate field. The formalism embraces features known from wave mechanics. Fourth, the field propagators are discussed, and are used to study reversibility in space.

Equilibrium Solution

By equilibrium we mean that $\dot{a}(x,t)$ in (2.14) is zero everywhere, with the condition that the system is isolated in the sense mentioned above. An

equilibrium solution, $a^0(x)$, therefore satisfies, for any x, and with zero current through all boundaries,

$$\int dy \Gamma(x,y) a^0(y) = \int dy \{G(x,y) a^0(y) - G(y,x) a^0(x)\} = 0, \qquad (3.1)$$

or $\overline{\overline{\Gamma}} \cdot \bar{a}^0 = 0$, in matrix notation. As indicated, we suppose that G is real and non-negative. The integration in (3.1) is the definite integral over the total system.

The original time-dependent function $a(x,t)$ was assumed to remain non-negative. If it tends towards an equilibrium function*, the latter must also be a non-negative function. In the present connection, however, we ask for all possible solutions $a^0(x)$ of (3.1). Equilibrium solutions $a^0(x)$ are real functions of x, because G is real.

We must verify at first that there is at least one solution of (3.1). We refrain from proving this for the widest possible groups of systems. The proof would, at this stage, be more cumbersome than rewarding. We need only demonstrate, by examples, that systems of interest have the required property. The general reason for this is seen easily for the group of finite discrete systems, i.e. for a finite discrete matrix $\overline{\overline{\Gamma}}$. In fact, conservation, (2.10), implies that $\bar{1} \cdot \overline{\overline{\Gamma}} = 0$, so that the determinant $|\overline{\overline{\Gamma}}| = 0$, and then eq. (3.1) must have at least one solution, irrespective of the symmetry properties of $\overline{\overline{G}}$.

The systems of the second major group are the following ones, with explicit solutions of (3.1). Suppose that the kernel in (3.1) is symmetric, $G(x,y) = G(y,x)$, or may be made symmetric by transformation of the space variables. The symmetric kernel $G(x,y)$ may then be taken outside the brackets in (3.1), and an equilibrium solution is $a^0(x) = \text{const.}$, or $\bar{a}^0 = C \cdot \bar{1}$. This solution is valid for all symmetric discrete or continuum cases, irrespective of the interval within which the system is defined. The symmetric case is analogous to a situation often met with in quantal or classical scattering. More precisely, the case of symmetric kernel $G(x,y)$ will be referred to as microscopic reversibility in space. It may be noted that equilibrium solutions can persist also in time dependent systems. If $G = G(x,y,t)$, and is symmetric, then $a^0(x) = \text{const.}$ is always an equilibrium.

A third simple group of systems consists of those with displacement invariance in space, $G(x,y) = G(x-y)$, cf. eq. (2.6). As to boundary conditions, one possibility is that a system is periodic (like e.g. angular vari-

* Note that in infinite space the function $a(x,t)$ will usually tend to zero everywhere, but it can tend to an equilibrium function $a^0(x)$ in the sense that $a(x,t)/a(x',t) \to a^0(x)/a^0(x')$.

ables), with repetition after a fixed, but arbitrarily long period. It is then obvious that $a^0(x) = \text{const.}$ is a solution of (3.1) for the system in question.

Beside the above group of systems one has a quite different group, consisting of communicating systems. Of these, a well-defined subgroup is the set of one-way systems, where for a discrete variable (e.g. $k = 1, 2, \ldots, N$, and $G_{kj} = C_k \cdot \delta_{k,j-1}$) a typical equilibrium solution is $a_1^0 = 1$, $a_2^0 = \ldots = a_N^0 = 0$.

Uniqueness of Equilibrium

Having ascertained that there is at least one equilibrium for the systems of interest, we propose to show the following result, valid for indivisible systems. Any solution of (3.1), if positive in one point, must be positive everywhere in x-space,

$$\text{indivisible systems: } a^0(x) > 0 \text{ for all } x. \tag{3.2}$$

Accept then that (3.2) holds and suppose that there are two or more equilibrium solutions. Any linear combination of these is also a solution of (3.1). But a linear combination can always be arranged to have both positive and negative values. This is in contradiction to (3.2). We have thus shown that (3.2) implies that there is exactly one equilibrium solution.

Let us now complete the proof by showing the validity of (3.2). We consider a system which is indivisible and isolated. Suppose that (3.2) is not fulfilled by $a^0(x)$, a solution of (3.1). Divide the space into region I where $a^0(x) > 0$, and region II where $a^0(x) \leq 0$. Integrate (3.1) over x within the whole region II. This integral is called Q, and must be zero according to (3.1). Now,

$$\left.\begin{aligned} Q &= \int_{\text{II}} dx \int dy \{G(x,y)a^0(y) - G(y,x)a^0(x)\} \\ &= \int_{\text{II}} dx \int_{\text{I}} dy \{G(x,y)a^0(y) - G(y,x)a^0(x)\}, \end{aligned}\right\} \tag{3.3}$$

because the symmetric part, where both y and x belong to II, is identically zero. Since $a^0(\text{II}) \leq 0$ we find by omitting the second term in (3.3)

$$Q \geqq \int_{\text{II}} dx \int_{\text{I}} dy G(x,y)a^0(y) > 0. \tag{3.4}$$

The latter inequality follows because $a^0(y)$ is positive everywhere, and $G(\text{II,I})$ must be different from zero for some set (x,y) in an indivisible

system. The resulting contradiction between eqs. (3.4) and (3.1) implies that (3.2) holds.

In the following we repeatedly use the result that, for indivisible systems, $a^0(x)$ is positive and equilibrium is unique. As to the properties of other systems, the communicating systems have not in general a unique equilibrium. In the special case of one-way systems there is uniqueness of equilibrium, but $a^0(x) = 0$ except in one point, so that (3.2) is not fulfilled.

Transformation to Normal Coordinates

For indivisible systems, with a unique, positive equilibrium solution $a^0(x)$, the quantity $a^0(x)\,dx = dz$ is a basic measure of a priori distribution, corresponding to phase space volume in statistical mechanics. It may then be worth while to indicate how the equation of motion can be transformed to suitable variables, i.e. normal coordinates, where the basic density measure is explicit. Still, it is not always necessary or convenient to make this transformation.

When transforming to the normal coordinates we find

$$a(x,t)\,dx = \frac{a(x,t)}{a^0(x)}\,a^0(x)\,dx = \alpha(z,t)\,dz. \tag{3.5}$$

Hereby we have obtained an invariant measure of the field,

$$\alpha(z,t) = \frac{a(x,t)}{a^0(x)}, \tag{3.6}$$

which function is well-defined, because $a^0(x)$ is positive. Usually, we consider α as a function in the z-space, but we may as well regard it as a function of x. The equilibrium solution $a^0(x)$ contains an arbitrary factor. If $a^0(x)$ is introduced as in eqs. (3.5) and (3.6), then α is normalized to unity because a is normalized.

The field equation for α is easily obtained. Define γ and g by

$$\left.\begin{aligned} \Gamma(x,y) &= a^0(x)\gamma(z,z'), \\ G(x,y) &= a^0(x)g(z,z'), \end{aligned}\right\} \tag{3.7}$$

where z and z' are the normal coordinates corresponding to x and y, respectively. Again, we may sometimes consider γ and g as explicit functions of x and y.

According to (2.9), (2.14), (3.5) and (3.7)

$$\dot{\alpha}(z,t) = \int dz'\gamma(z,z')\alpha(z',t) = \int dz'\{g(z,z')\,\alpha(z',t) - g(z',z)\alpha(z,t)\}, \tag{3.8}$$

where then, from conservation (2.10),

$$\int dz\gamma(z,z') = 0, \tag{3.9}$$

and from (3.1)

$$\int dz'\gamma(z,z') = \int dz'\{g(z,z') - g(z',z)\} = 0, \tag{3.10}$$

corresponding to equilibrium being the uniform distribution.

As to the field conjugate to $\alpha(z,t)$, we denote it as $\beta(z,t)$ and can simply introduce

$$\beta(z,t) = b(x,t), \tag{3.11}$$

i.e. $\beta(z,t)\,dz = b(x,t)\,a^0(x)\,dx$, so that from (2.20)

$$\dot{\beta}(z,t) = -\int dz'\beta(z',t)\gamma(z',z) = -\int dz'\{\beta(z',t) - \beta(z,t)\}g(z',z). \tag{3.12}$$

Eqs. (3.12) and (3.8) show that $\beta(z,t)$ (or $b(x,t)$) is in fact the field conjugate to $\alpha(z,t)$, in the same way as (2.20) is conjugate to (2.13).

It is apparent that, because $a(x,t)$ has an equilibrium, the conjugate field has conservation. In fact, according to eqs. (3.12) and (3.10)

$$\int a^0(x)\,\dot{b}(x,t)\,dx = \int dz\dot{\beta}(z,t) = 0. \tag{3.13}$$

Trend towards Equilibrium

The trend towards equilibrium is easily found if, by means of (3.10) the equation of motion (3.8) is written in an alternative way,

$$\dot{\alpha}(z,t) = \int dz'g(z,z')\{\alpha(z',t) - \alpha(z,t)\}. \tag{3.8'}$$

Eq. (3.8′) is seen to be quite similar to (3.12). It follows from (3.8′) that the largest value of $\alpha(x,t)$ must always decrease, whereas the smallest value, if any, must increase. This indicates a tendency towards equilibrium, cf. also § 4. The result remains valid if the function α in (3.8′) is allowed to be negative.

For the conjugate field already the original equation of motion (2.20) implies that the largest value of $b(x,t)$ decreases, and the smallest increases, as one goes backwards in time.

Eigenvalues and Eigenfunctions

The equilibrium solution $a^0(x)$ in (3.1) is merely one of the stationary solutions of (2.14), albeit the most important one. Consider now stationary solutions in general, for isolated, indivisible systems. Make the ansatz that a solution of (2.14) is of the type $a_\nu(x)\cdot\exp(-\lambda_\nu t)$, i.e. the equation becomes

$$\lambda_\nu a_\nu(x) = -\int dy \Gamma(x,y) a_\nu(y) \quad \text{or} \quad \lambda_\nu \overline{a_\nu} = -\overline{\overline{\Gamma}} \cdot \overline{a_\nu}. \tag{3.14}$$

The equilibrium solution corresponds to $\lambda_0 = 0$. In parallel to (3.14) we may directly consider the invariant field α, where

$$\left.\begin{aligned} &\lambda_\nu \alpha_\nu(z) = -\int dz' \gamma(z,z') \alpha_\nu(z') = -\int dz' g(z,z')(\alpha_\nu(z') - \alpha_\nu(z)) \\ &\text{or} \\ &\lambda_\nu \overline{\alpha}_\nu = -\overline{\overline{\gamma}} \cdot \overline{\alpha}_\nu. \end{aligned}\right\} \tag{3.15}$$

The result obtained from (3.8′) proves, firstly, that for the non-equilibrium stationary solutions it must hold that

$$\mathrm{Re}(\lambda_\nu) > 0, \tag{3.16}$$

because for no function $\alpha(z,t)$ is there a tendency away from equilibrium. Secondly, since $a(x,t)$ is conserved, these eigensolutions obey the equation, for $\nu \neq 0$,

$$\int a_\nu(x)\, dx = \int \alpha_\nu(z)\, dz = \bar{\alpha}_\nu \cdot \overline{1} = 0. \tag{3.17}$$

The result (3.17) is part of a more general orthogonality theorem. We prove the theorem in two steps. First, we consider the limited, but common, case of symmetric kernels (microscopic reversibility in space, cf. p. 19). Next, we give the proof in the general case.

Suppose then that $\overline{\overline{\gamma}}$ is symmetric, $\gamma(z,z') = \gamma(z',z)$, and use matrix notation for brevity. Prove first that the λ_ν are real. The complex conjugate of eq. (3.15) is $\lambda_\nu^* \bar{\alpha}_\nu^* = -\overline{\overline{\gamma}} \cdot \bar{\alpha}_\nu^*$. Multiply (3.15) by $\bar{\alpha}_\nu^*$ on the left

$$\lambda_\nu \bar{\alpha}_\nu^* \cdot \bar{\alpha}_\nu = -\bar{\alpha}_\nu^* \cdot \overline{\overline{\gamma}} \cdot \bar{\alpha}_\nu = -\bar{\alpha}_\nu \cdot \overline{\overline{\gamma}}^T \cdot \bar{\alpha}_\nu^* = -\bar{\alpha}_\nu \cdot \overline{\overline{\gamma}} \cdot \bar{\alpha}_\nu^* = \lambda_\nu^* \bar{\alpha}_\nu^* \cdot \bar{\alpha}_\nu, \tag{3.18}$$

so that $\lambda_\nu^* = \lambda_\nu$, and therefore the eigenfunctions $\bar{\alpha}_\nu = \alpha_\nu(z)$ may be chosen to be real.

Prove next, also for symmetric $\overline{\overline{\gamma}}$, that eigensolutions belonging to different λ_ν are orthogonal. Introduce two eigenfunctions, $\bar{\alpha}_\nu$ and $\bar{\alpha}_\mu$. Multiply (3.15) by $\bar{\alpha}_\mu$,

$$\lambda_\nu \bar{\alpha}_\mu \cdot \bar{\alpha}_\nu = -\bar{\alpha}_\mu \cdot \overline{\overline{\gamma}} \cdot \bar{\alpha}_\nu = -\bar{\alpha}_\nu \cdot \overline{\overline{\gamma}}^T \cdot \bar{\alpha}_\mu = \lambda_\mu \bar{\alpha}_\mu \cdot \bar{\alpha}_\nu, \tag{3.19}$$

$\overline{\overline{\gamma}}^T$ being the transposed matrix. It follows that

$$\bar{\alpha}_\mu \cdot \bar{\alpha}_\nu = 0 \quad \text{for} \quad \lambda_\mu \neq \lambda_\nu, \quad \text{if} \quad \overline{\overline{\gamma}}^T = \overline{\overline{\gamma}}. \tag{3.20}$$

In the symmetric case, the $\bar{\alpha}_\nu$ may therefore form an orthonormal set.

For the purpose of studying the general orthogonality theorem we introduce the conjugate field. We define its eigenfunctions as $b_\nu(x) \cdot \exp(\lambda_\nu t)$, so that, corresponding to (3.14),

$$\bar{b}_\nu \lambda_\nu = -\bar{b}_\nu \cdot \bar{\bar{\Gamma}}. \tag{3.21}$$

We multiply (3.14) by $\bar{b}_\mu$ and obtain

$$\lambda_\nu \bar{b}_\mu \cdot \bar{a}_\nu = -\bar{b}_\mu \cdot \bar{\bar{\Gamma}} \cdot \bar{a}_\nu = \lambda_\mu \bar{b}_\mu \cdot \bar{a}_\nu. \tag{3.22}$$

It follows that

$$\bar{b}_\mu \cdot \bar{a}_\nu = 0 \quad \text{if} \quad \lambda_\mu \neq \lambda_\nu. \tag{3.23}$$

This result is quite general. It is independent of the previous results in this chapter, such as $a^0(x) > 0$. It is valid not only for the original equations of motion (2.14) and (2.20), but even when $G(x,y)$ is allowed not to be real and positive. In fact, (3.23) is a consequence of merely the first, fourth, and fifth constraints, i.e. (2.9) with $\Gamma = \Gamma(x,y)$.

According to eq. (3.23) the eigenfunctions $a_\nu(x)$ do not in general form an orthonormal set. They do it when, as in eq. (3.20), $\bar{a}_\nu = \bar{b}_\nu$.

If we can normalize and may assume non-degeneracy, we obtain from (3.23)

$$\int b_\mu(x) a_\nu(x) dx = \delta_{\mu\nu}. \tag{3.24}$$

For a function $f(x)$ the coefficients of an expansion

$$f(x) = \sum_\nu c_\nu a_\nu(x), \tag{3.25}$$

are according to (3.24)

$$c_\nu = \int b_\nu(x) f(x) dx. \tag{3.26}$$

Although it would be easy, we shall at this point not enter into further details of the formulation by eigenfunctions, as based only on eqs. (2.1), (2.4) and (2.5). It is apparent that the present formalism is quite as in quantum mechanics, the latter being in fact embraced by the former. As an example one might consider stationary perturbation theory. Perturbation theory is useful when one knows exact solutions of many cases of equations of motion, the neighbouring cases being then easily approximated. The examples of analytic solutions discussed in § 6 can in this respect serve as a basis, both for indivisible systems and for, e.g., one-way systems.

Propagators

We introduced in (2.7) the propagator $T(x,t;\ x',t')$ as an expression for the integrated equation of motion, such that

$$a(x,t) = \int dx' T(x,t;\ x',t') a(x',t'), \tag{3.27}$$

where, for $t = t'$, $T = \delta(x - x')$. The propagator is defined for $t \geq t'$, but not necessarily for $t < t'$.

The equations of motion for the propagator are obtained from (3.27) by differentiation with respect to the time variables. Differentiate first (3.27) with respect to t, and find from (2.9), since $a(x', t')$ may be chosen arbitrarily,

$$\frac{\partial}{\partial t} T(x, t; x', t') = \int dy \Gamma(x, y, t)\, T(y, t; x', t'), \tag{3.28}$$

or $\frac{\partial}{\partial t} \overline{\overline{T}}(t, t') = \overline{\overline{\Gamma}}(t) \cdot \overline{\overline{T}}(t, t')$, i.e. again the equation of motion (2.9). Similarly, we differentiate (3.27) with respect to t' and obtain

$$\frac{\partial}{\partial t'} T(x, t;\ x', t') = -\int dy T(x, t;\ y, t') \Gamma(y, x', t'). \tag{3.29}$$

We have hereby seen the significance of the equation of motion for the conjugate field, (2.20), the latter being identical to (3.29).

The above concerned the propagation of a field, cf. (3.27). The propagation of the conjugate field is evidently determined by

$$b(x', t') = \int dx\, b(x, t) T(x, t;\ x', t'), \tag{3.30}$$

or $\overline{b}(t') = \overline{b}(t) \cdot \overline{\overline{T}}(t, t')$.

If we specialize to the case of time-independent equations of motion, i.e. the fifth constraint, or (2.14), we get from (3.27)

$$T = T(x, x', t - t') = T(x, x', \tau), \tag{3.31}$$

the propagator being dependent on only the time difference $\tau = t - t'$, and defined at least for $\tau \geq 0$. It follows that then

$$\frac{\partial}{\partial \tau} \overline{\overline{T}}(\tau) = \overline{\overline{T}}(\tau) \cdot \overline{\overline{\Gamma}} = \overline{\overline{\Gamma}} \cdot \overline{\overline{T}}(\tau) = \tfrac{1}{2} [\overline{\overline{T}}(\tau) \cdot \overline{\overline{\Gamma}} + \overline{\overline{\Gamma}} \cdot \overline{\overline{T}}(\tau)], \tag{3.32}$$

the change of T being determined by its anticommutator with Γ.

The equation of motion of the transposed T-matrix is

$$\frac{\partial}{\partial \tau} \overline{\overline{T}}^{T}(\tau) = \tfrac{1}{2} [\overline{\overline{\Gamma}}^{T} \cdot \overline{\overline{T}}^{T}(\tau) + \overline{\overline{T}}^{T}(\tau) \cdot \overline{\overline{\Gamma}}^{T}], \tag{3.33}$$

being thus governed by the transposed Γ-matrix.

Reversibility in Space

Let us consider transitions in space during finite times. For definiteness, suppose that at time t_1 the field is $a(x,t_1) = \delta(x - x_1)$. Ask for the field at time t_2 in the point x_2, $a(x_2,t_2)$, and call this field the transition rate $P_a(x_1 \to x_2, t_1 \to t_2)$. According to (3.27) the transition rate is given by the propagator

$$P_a(x_1 \to x_2,\ t_1 \to t_2) = T(x_2,t_2;x_1,t_1),$$

and analogously for the conjugate field, cf. (3.30),

$$P_b(x_1 \to x_2,\ t_1 \to t_2) = T(x_1,t_1;\ x_2,t_2).$$

It follows that

$$P_a(x_1 \to x_2,\ t_1 \to t_2) = P_b(x_2 \to x_1,\ t_2 \to t_1). \tag{3.34}$$

The formula (3.34) is in fact of quite general validity, in that it states: If P_a is defined for a transition, then P_b of the opposite transition is also defined and equal to it.

Consider next time-independent equations of motion. According to (3.31), eq. (3.34) becomes

$$P_a(x_1 \to x_2,\tau) = P_b(x_2 \to x_1,-\tau) = T(x_2,x_1,\tau), \tag{3.35}$$

where $\tau = t_2 - t_1$.

Finally, we suppose that there is microscopic reversibility in space, i.e. we are concerned with z-space, where $\gamma(z_1,z_2) = \gamma(z_2,z_1)$. The a- and b-fields in z-space are called α and β. It is now observed that since $\bar{\bar{\gamma}}^T = \bar{\bar{\gamma}}$, the equations of motion (3.32) and (3.33) for $\bar{\bar{T}}(\tau)$ and $\bar{\bar{T}}^T(\tau)$ are identical. Since the initial value is symmetrical, $\bar{\bar{T}}(0) = \bar{\bar{T}}^T(0) = \delta(z_2 - z_1)$, it follows that $\bar{\bar{T}}(\tau) = \bar{\bar{T}}^T(\tau)$, or from (3.35)

$$P_\alpha(z_1 \to z_2,\tau) = P_\alpha(z_2 \to z_1,\tau) \tag{3.36}$$

and this again is equal to $P_\beta(z_2 \to z_1,\ -\tau) = P_\beta(z_1 \to z_2,\ -\tau)$. Eq. (3.36) states that if there is microscopic reversibility in space, then macroscopic reversibility in space follows. The result is valid in the same strong sense as (3.34). A transformation of (3.36) to arbitrary coordinates yields

$$\frac{P_a(x_1 \to x_2,\tau)}{a^0(x_2)} = \frac{P_a(x_2 \to x_1,\tau)}{a^0(x_1)}, \tag{3.36'}$$

so that transition rates are weighted by the equilibrium distribution.

§ 4. Degradation Functions

The concept of entropy and the properties of entropy are familiar from statistical mechanics and from thermodynamics. The present integral equations contain main features of statistical mechanics. One might therefore be tempted to introduce entropy as a recipe, without further ado, thus obtaining a measure of the degradation of the field within a system. This is in fact a possible procedure. It appears the more plausible since entropy also plays a central role in the mathematical theory of information[9, 19].

But in the present discussion we need not rely on concepts derived from applications. It seems therefore worth while to attempt independently a general formulation of the concept in question. We shall do this in the beginning of the present chapter. We arrive at the noteworthy result that entropy represents merely one choice within a family of degradation functions. Next, we briefly discuss the use of degradation functions as describing the trend towards equilibrium. It appears that entropy often is not the most convenient choice of degradation function.

Basic Requirements

We ask for a universal quantity characterizing the state of a system. A quantity of this kind we call a degradation function. We make the following two demands, to be explained presently in more detail:

1. A degradation function must be unique, invariant, and common to indivisible systems.
2. A degradation function must have a well-defined rule of composition for a system consisting of two completely independent systems.

Consider the first demand. The stipulation of uniqueness has a straightforward meaning. As to invariance, this means that a degradation function remains unchanged, whatever transformation is made of the spatial coordinates of a system. Thirdly, we express the desired universality of the degradation function by requiring explicitly that it is common to indivisible systems. Indivisible systems form an exceedingly wide group, with the property of unique and positive equilibrium distribution. It may turn out that degradation functions apply for a still wider group of systems, but we need not mince matters by going beyond indivisible systems.

A degradation function must be of type of the projections introduced in § 2. They are of two kinds: projections of spatial functions, $\langle f(x) \rangle$ in (2.16), and projections of functions of the field, $\langle q(a) \rangle$ in (2.17). In these

integrals the differential $dP = a(x,t)\,dx$ is invariant, and thus $f(x)$ and $q(a)$ must be invariant too.

It is not particularly difficult to ascertain that projections of spatial functions do not fulfill the above demands. Without going into detail, we may briefly indicate some of the main aspects. One would expect that $f(x)$ is a function given beforehand, independently of the equations of motion of the system in question. Now, since $f(x)$ is invariant, it may be expressed by the invariant b-field, i.e. in terms of its complete set of eigenfunctions $b_\nu(x)$. But if $f(x)$ is to be independent of the equations of motion, there remains only the uninteresting choice $f(x) = b_0(x) = \text{const}$. On the other hand, if f were allowed to depend on the equations of motion, it could not be unique and common to all systems within discrete or continuum spaces.

Let us turn to functions of the field. In order to secure invariance we must introduce the invariant field $\alpha = a(x,t)/a^0(x)$, defined in (3.5). It exists for any indivisible system. The only quantities fulfilling the first demand are therefore, expressed in normal coordinates,

$$D(t) = \langle q(\alpha)\rangle = \int dz\,\alpha(z,t)\,q(\alpha(z,t)), \tag{4.1}$$

where $q(\alpha)$ is arbitrary, so far.

Introduce now the second demand. Suppose that the physical quantity in question is D_1 and D_2 for two independent systems, and that it is D_{12} for the two taken together. The demand is then that there is a well-defined rule of composition,

$$D_{12} = G(D_1, D_2). \tag{4.2}$$

This demand is often implicitly made by introduction of physical variables, sometimes as a more incautious statement of additivity or superposition.

Before applying (4.2) we consider the notion of independent systems. Let there be two systems, described in normal coordinates by the fields $\alpha_1(z_1,t)$ and $\alpha_2(z_2,t)$. The systems are independent if $\alpha_1(z_1,t)$ and $\alpha_2(z_2,t)$ separately account for their future behaviour. The two systems can also be considered as one system with a field $\alpha(z_1,z_2,t)$, if

$$\alpha(z_1, z_2, t) = \alpha_1(z_1, t)\,\alpha_2(z_2, t), \tag{4.3}$$

where the fields are normalized to unity.

The second demand, (4.2), can now be formulated by means of (4.1) and (4.3). For the total system one has

$$D_{12} = \langle q(\alpha(z_1,z_2,t))\rangle = \int dz_1 \int dz_2 \alpha(z_1,z_2,t) q(\alpha(z_1,z_2,t)), \tag{4.4}$$

and for the individual systems

$$\left.\begin{aligned} D_1 &= \langle q(\alpha_1(z_1,t))\rangle_1 = \int dz_1 \alpha_1(z_1,t)\, q(\alpha_1(z_1,t)), \\ D_2 &= \langle q(\alpha_2(z_2,t))\rangle_2 = \int dz_2 \alpha_2(z_2,t)\, q(\alpha_2(z_2,t)). \end{aligned}\right\} \tag{4.5}$$

The solutions of eqs. (4.2), (4.3), (4.4) and (4.5) may be readily guessed. Let us indicate a more systematic procedure. Put $\alpha_2(z_2,t) = \xi = \text{const.}$ in one region of z_2-space, and $\alpha_2 = 0$ outside this region. Eq. (4.2) then becomes, according to eqs. (4.3), (4.4), and (4.5),

$$\langle q(\xi\alpha_1)\rangle_1 = G(\langle q(\alpha_1)\rangle_1, q(\xi)). \tag{4.6}$$

In eq. (4.6) we next vary $\alpha_1(z_1)$, retaining normalization of α_1 and keeping $\langle q(\alpha_1)\rangle_1$ constant. Since G is then unchanged, also $\langle q(\xi\alpha_1)\rangle_1$ must remain unchanged. Introducing $Q(\alpha) = \partial(\alpha q(\alpha))/\partial\alpha$, one obtains, by variation of α_1, the functional equation $Q(\xi\alpha_1) = C_1(\xi)Q(\alpha_1) + C_2(\xi)$, which may be solved ($Q(\alpha) \propto c + \alpha^n$ or $c + \log\alpha$). A precise discussion of the functional equation is given in ref. 2.

The solutions for q are then

$$q(\alpha) = C\alpha^n \quad \text{and} \quad q(\alpha) = -C\log\alpha, \tag{4.7}$$

the latter solution being due to the normalization condition for α, i.e. to conservation of the field. We have in (4.7) omitted a spurious solution, $q(\alpha) = C\alpha^{-1}\log\alpha$, for which the projection often diverges, in particular within an infinite system.

We have thus arrived at the family of functions satisfying the two demands. We call them degradation functions, writing

$$D^{(n)}(t) = \int dz \alpha(z,t)[\alpha(z,t)]^n, \tag{4.8}$$

and denoting by S the familiar entropy,

$$S(t) = -\int dz \alpha(z,t)\log\alpha(z,t), \tag{4.9}$$

where the arbitrary constants in eq. (4.7) are omitted. The number n in eq. (4.8) is the order of the D-function. If one limits the order to be $n \geq 0$, convergence is always secured.

The value $n = 0$ in (4.8) is the trivial normalization. Note here that the entropy, (4.9), which arose from conservation of the field, is the derivative of a D-function,

$$S = -\frac{\partial}{\partial n} D^{(n)}\bigg|_{n=0} = -\frac{1}{n}\log D^{(n)}\bigg|_{n\to 0} = -\frac{D^{(n)}-1}{n}\bigg|_{n\to 0}. \tag{4.10}$$

Entropy is thus a degradation function of order zero.

It follows from eqs. (4.9) and (4.8) that when a system is composed of independent systems, then the entropy is additive, as is also the logarithm of the D-functions,

$$\left.\begin{aligned} \log D_{12}^{(n)} &= \log D_1^{(n)} + \log D_2^{(n)}, \\ S_{12} &= S_1 + S_2. \end{aligned}\right\} \tag{4.11}$$

Strictly speaking, only the changes of the quantities in (4.11) are well-defined. This is because they contain an arbitrary additive constant in a continuum description, arising from an arbitrary factor in the definition of z, whereas αdz is invariant. The arbitrary constant is removed in the case of a discrete variable with finite N. This contrast is well-known for entropy in classical statistical mechanics as compared with quantal statistical mechanics.

The likeness between entropy and the D-functions, as contained in eqs. (4.11) and (4.10), may be further elucidated by introducing a set of functions $S^{(n)}$,

$$S^{(n)} = -\frac{1}{n} \log D^{(n)}. \tag{4.12}$$

According to eq. (4.10), $S^{(0)} = S$. Moreover, consider the example of a discrete variable, $k = 1, 2, \ldots, N$, with equilibrium $\alpha_1^0 = \alpha_2^0 = \ldots = \alpha_N^0 = 1/N$. In an initial state, where one α_k is unity, the others zero, we find that all functions in (4.12) are $S^{(n)} = 0$. In the final equilibrium they are all $S^{(n)} = \log N$. Between the two extremes the different functions attain quite different values. The equality of the functions at the extremes is only due to the freedom in selection of origin and in unit of degradation. The likeness may, however, be one reason why attempts at deducing degradation functions from general principles have led only to the entropy, omitting the D-functions.

Monotonic Change in Time of Degradation Functions

We now apply the linear integral equations of motion, in order to find the time behaviour of the degradation functions. It will be shown that for indivisible systems the D-functions always decrease, when the field deviates from the equilibrium solution. According to (3.8) and (3.10) we can write the equation of motion as

$$\dot{\alpha}(z,t) = \int dz' \{ g(z,z') \alpha(z',t) - \alpha(z,t)(Cg(z',z) + (1-C) g(z,z')) \}, \tag{4.13}$$

where C is an arbitrary constant.

The time derivative of the function $D^{(n)}(t)$ is therefore, according to (4.8),

$$\left.\begin{aligned}\frac{\partial}{\partial t}D^{(n)}(t) = (n+1)\int dz\int dz' g(z,z')\{\alpha(z',t)\alpha^n(z,t) - \\ - C\alpha^{n+1}(z',t) - (1-C)\alpha^{n+1}(z,t)\}.\end{aligned}\right\} \tag{4.14}$$

In this equation we can choose the constant to be $C = (n+1)^{-1}$. Next we introduce an auxiliary function

$$f_n(\xi) = (n+1)(\xi - 1) + 1 - \xi^{n+1}, \qquad 0 \leq \xi < \infty, \tag{4.15}$$

with the property $f_n(1) = 0$, while $f_n(\xi) < 0$ for $\xi \neq 1$ and $n > 0$.

In eq. (4.14) the function $\alpha^{n+1}(z,t)$ is taken outside the brackets, so that

$$\frac{\partial}{\partial t}D^{(n)}(t) = \int dz\int dz' g(z,z')\alpha^{n+1}(z,t) f_n\left(\frac{\alpha(z',t)}{\alpha(z,t)}\right). \tag{4.16}$$

Within the family of degradation functions, the time behaviour of the first order D-function is particularly simple for linear equations of motion. We specify (4.16) in this case

$$\frac{\partial}{\partial t}D^{(1)}(t) = -\int dz\int dz' g(z,z')\{\alpha(z,t) - \alpha(z',t)\}^2, \tag{4.16'}$$

where we can replace $g(z,z')$ by $g^s(z,z') = (g(z,z') + g(z',z))/2$. Moreover, $D^{(1)}$ itself has a simple geometric interpretation, $D^{(1)} = \bar{\alpha}\cdot\bar{\alpha}$, being thus the square of the vector $\bar{\alpha}$, for which $\bar{1}\cdot\bar{\alpha} = 1$.

It can be readily concluded from eq. (4.16), because of the properties of $f_n(\xi)$, that for indivisible systems, and for $n > 0$,

$$\frac{\partial}{\partial t}D^{(n)}(t) < 0, \text{ unless} \frac{\alpha(z',t)}{\alpha(z,t)} = 1 \text{ for all } z,\ z'. \tag{4.17}$$

In fact, suppose that $\dot{D}^{(n)}(t) = 0$. Consider an arbitrary point z_a, where $\alpha = \alpha(z_a,t)$. According to eq. (4.16), all points z_1 for which $g^s(z_a,z_1) \neq 0$ must have $\alpha(z_1,t) = \alpha(z_a,t)$. The points z_1 communicate directly with other points z_2 which must have the same value of α. Since the system is indivisible, the arbitrary point z_a must communicate in this way with any other point z_b, such that $\alpha(z_a,t) = \alpha(z_b,t)$, from which follows eq. (4.17).

We have thus proved that all D-functions decrease monotonically towards their equilibrium value. The monotonic behaviour of entropy is also a consequence of (4.17). To be precise, the time derivative of entropy is

according to (4.10) obtained from (4.16) by division with n, letting $n \to 0$, whereby, in the integrand, $f_n/n \to f = \xi - 1 - \xi \log \xi$, i.e. one obtains the auxiliary function of Gibbs[7].

Several conclusions may be drawn from (4.17). It follows, for instance, that any non-uniform function in z-space, normalized to unity, has a higher value of $D^{(n)}$ than the normalized uniform distribution, for any $n > 0$. Further, we have proved previously that there is only one equilibrium of the linear equations of motion. It does, however, also follow from (4.17) that there could be no equilibrium solution other than the uniform distribution, because $\partial D^{(n)}/\partial t \neq 0$ for all other distributions.

§ 5. Connection to Differential Equations

We consider differential equations of first order in time and of first or higher order in space. Such differential equations have merits on their own, and can be considered as possible equations of motion obeying the constraints. Apart from this, they are often useful approximations to integral equations, and in diffusion phenomena they even lead to quite accurate solutions. The familiar approximation involved in a differential equation is that $G(x,y)$ is negligible unless $|x - y|$ is small. By expansion one may then obtain a differential equation in x, usually of second order.

We briefly discuss the limitations put on a differential equation by the constraints in § 2. It turns out that differential equations can be of, at most, second order in space. The differential equations imply a trend towards equilibrium, with the notable exception of first order equations. We finally study the symmetry properties of the diffusion equation, and its use as an approximation to the integral equation.

Basic Structure

When trying to find the possible structure of differential equations, one might start from the basic integral equation, (2.13). We prefer to use the equivalent procedure of introducing the initial four constraints of § 2. In order to have simplicity of notation we consider the one-dimensional case. According to the first and fourth constraints, (2.1) and (2.4), we demand that, if the derivatives $\partial^n a(x,t)/\partial x^n$ are given, then the time derivative $\dot{a}(x,t)$ is known, being linear in the spatial derivatives. To finite order, N, we therefore find

$$\dot{a}(x,t) = \sum_{n=0}^{N} \lambda_n(x,t) \frac{\partial^n}{\partial x^n} a(x,t). \tag{5.1}$$

In order to retain conservation explicitly, i.e. the second constraint, (2.2), we introduce $\dot{a}(x,t)$ as minus the divergence of the current density, (2.23),

$$\dot{a}(x,t) = -\frac{\partial}{\partial x} j(x,t), \tag{5.2}$$

expanding the current in spatial derivatives of $a(x,t)$,

$$j(x,t) = -\sum_{n=0}^{N-1} \Lambda_n(x,t) \frac{\partial^n}{\partial x^n} a(x,t). \tag{5.3}$$

The number of independent functions in (5.2), (5.3) is one less than in (5.1), giving the condition on the λ_n's,

$$\lambda_n(x,t) = \frac{\partial}{\partial x} \Lambda_n(x,t) + \Lambda_{n-1}(x,t), \tag{5.4}$$

with $\Lambda_N = 0$.

The freedom in the above scheme is strongly reduced by the third constraint, (2.3), demanding that a non-negative $a(x,t)$ remains non-negative at all later times. Suppose therefore that $a(x,t) = 0$, and accordingly $a'(x,t) = 0$, $a''(x,t) \geq 0$. It should then follow that $\dot{a}(x,t) \geq 0$. This places no restrictions on $\lambda_0(x,t)$ or $\lambda_1(x,t)$, but $\lambda_2(x,t)$ must remain non-negative, $\lambda_2(x,t) \geq 0$.

Consider next the possibility of a differential equation of finite order N, i.e. (5.1), with $N > 2$. We may suppose that, at a given time $t = 0$,

$$a(x, t = 0) = \frac{(x + C_N x^{N-1})^2 + x^{2N-2}}{1 + c^2 x^{2N}}. \tag{5.5}$$

This function is normalizable and it is positive everywhere, except at the origin, where $a(0,0) = 0$, $a^{(N)}(0,0) = 2C_N \cdot N!$, all lower spatial derivatives, except $a''(0,0) = 2$, being zero. Therefore $\dot{a}(x = 0, t = 0) = \lambda_2 \cdot 2 + \lambda_N \cdot 2C_N N!$, and since C_N may be chosen arbitrarily, the coefficient λ_N in (5.1) must be $\lambda_N = 0$, in order to fulfill always $\dot{a}(0,0) \geq 0$. The differential equation (5.1) therefore cannot be of higher than second order, if it obeys merely the first and third constraints. If we assume conservation, (5.2), we can only be concerned with the diffusion equation, or Fokker-Planck equation,

$$\dot{a}(x,t) = \frac{\partial}{\partial x} D(x,t) \frac{\partial}{\partial x} a(x,t) - \frac{\partial}{\partial x} w(x,t) a(x,t), \tag{5.6}$$

with the current $j(x,t) = -D(x,t)a'(x,t) + w(x,t)a(x,t)$, and where $D(x,t) \geq 0$.

In the case of multi-dimensional space the proof is completely analogous to the above one. The result is that one can only permit the following equation

$$\dot{a}(\vec{x},t) = \sum_{i,k} \frac{\partial}{\partial x_i} D_{ik}(\vec{x},t) \frac{\partial}{\partial x_k} a(\vec{x},t) - \sum_i \frac{\partial}{\partial x_i} w_i(\vec{x},t) a(\vec{x},t). \qquad (5.7)$$

where the matrix D_{ik} at any space-time point has non-negative eigenvalues, like D in (5.6), because $\dot{a}$ must be non-negative when $a = 0$. Note that we can always choose the matrix to be symmetric, $D_{ik}(\vec{x},t) = D_{ki}(\vec{x},t)$. With this choice there is a unique separation between the two terms in (5.7).

The impossibility of spatial derivatives of higher than second order is rather remarkable. It does not seem to be explicitly noted in connection with derivations of diffusion approximations. On the contrary, it is sometimes stated that higher order terms in an expansion are small and can be disregarded[5], or it is attempted to introduce explicitly a term of higher order[10] (cf. also ref. 18, p. 238).

The above result shows that differential equations are not very flexible, and can hardly be expected to represent even the main general features of the basic integral equation. Quite apart from this conclusion, the actual kernels $G(x,y)$ with which we shall be concerned (cf. § 6) will often decrease comparatively slowly for $|x-y| \to \infty$, leading to e.g. a divergent moment $\langle x^2 \rangle$ of the distribution. This does not fit in with a diffusion equation.

The equation for the conjugate field corresponding to (5.7) is easily obtained from (3.27)—by differentiation with respect to t'—

$$\dot{b}(\vec{x},t) = -\sum_{i,k} \frac{\partial}{\partial x_i} D_{ki}(\vec{x},t) \frac{\partial}{\partial x_k} b(\vec{x},t) - \sum_i w_i(\vec{x},t) \frac{\partial}{\partial x_i} b(\vec{x},t). \qquad (5.8)$$

The first operator in (5.8) is equal to minus the first operator in (5.7) if D_{ik} is symmetric. The second operator in (5.8) is equal to the second one in (5.7), provided $\operatorname{div} \vec{w} = 0$.

Let us finally note that the diffusion equation may be considered as a singular operator to be added to the integral equation, because it only results from an integral equation by a limiting process. The integral equation (2.13), with a continuous $G(x,y,t)$, we denote as $\dot{a} = \vartheta_i(t)a$. Similarly, the diffusion equation (5.7) is $\dot{a} = \vartheta_d(t)a$. Within the present context the most general equation of motion, obeying the first four constraints, is $\dot{a} = \vartheta_i(t)a + \vartheta_d(t)a$.

Trend towards Equilibrium; Reversibility

We have previously shown, in §§ 3 and 4, that all systems with one equilibrium $a^0(x) > 0$ tend towards this equilibrium if, in the integral equation, $G(x,y)$ does not vanish for all $y \neq x$. The diffusion equations constitute a somewhat singular limiting case. Let us consider the trend towards equilibrium by means of the degradation functions.

We may suppose, without essential loss of generality, that in (5.7) the equilibrium function $a^0(\vec{x})$ is a constant, corresponding to normal coordinates,

$$a^0(\vec{x}) = \text{const., i.e. } \operatorname{div} \vec{w}(\vec{x}) = 0. \tag{5.9}$$

The latter equation shows that $a(\vec{x},t)$ corresponds to the density of an incompressible liquid.

From (5.7) and (4.8) we find directly in a space of m dimensions,

$$\left.\begin{aligned} \frac{\partial}{\partial t} D^{(n)}(t) &= \frac{\partial}{\partial t} \int^{(m)} dx\ (a(\vec{x},t))^{n+1} \\ = (n+1) \int^{(m)} dx\ a^n(\vec{x},t) \left\{ \sum_{i,k} \frac{\partial}{\partial x_i} D_{ik}(\vec{x},t) \frac{\partial}{\partial x_k} a(\vec{x},t) - \sum_i \frac{\partial}{\partial x_i} w_i(\vec{x},t) a(\vec{x},t) \right\} \\ = -\sum_{i,k} (n+1) n \int^{(m)} dx\ a^{n-1}(\vec{x},t) D_{ik}(\vec{x},t) \frac{\partial a(\vec{x},t)}{\partial x_i} \frac{\partial a(\vec{x},t)}{\partial x_k} \leq 0, \end{aligned}\right\} \tag{5.10}$$

where we use that the current vanishes at the boundaries, or that the system is periodic. The equality sign in (5.10) holds only in equilibrium for an indivisible system, for positive eigenvalues of D_{ik}.

The proper diffusion equation is thus irreversible, like the integral equation. Still, there remains one singular exception since, if $D_{ik} = 0$ everywhere, all degradation functions remain constant. The remaining reversible first order equations, fulfilling (5.9) for indivisible systems, are

$$\dot{a}(\vec{x},t) = -\operatorname{div}[\vec{w}(\vec{x},t) a(\vec{x},t)], \quad \operatorname{div} \vec{w}(\vec{x},t) = 0. \tag{5.11}$$

It follows from (5.8) that the conjugate field also obeys (5.11). The eigenvalues λ_n of (5.11) are purely imaginary and, as mentioned, all degradation functions are constant in time.

Eq. (5.11) is just of the kind with which one is concerned in a Hamiltonian description of the motion of an ensemble in classical phase space, with $\vec{x} = (x_1, \ldots, x_{2N}) = (q_1, \ldots, q_N, p_1, \ldots, p_N)$. The Hamiltonian equations of motion are inconveniently singular, in the sense that the least deviation from (5.11) brings about irreversibility.

It may be noted that the first order equation of motion (5.11) is the only possible one, if the first constraint is tightened. In fact, when the first four constraints are valid, the general equations (2.13) follow. Suppose here that the first constraint (2.1) is modified by the demand that $a(x',t')$ is determined by $a(x,t)$ not only for $t' > t$, but also for $t' < t$. It follows that for $x \neq y$ the kernel $G(x,y,t)$ is both non-negative (from $t' > t$) and non-positive (from $t' < t$). We are then left with the singular case of infinitely narrow G, i.e. the differential equation (5.7). But here, again, the eigenvalues of D_{ik} must be both non-negative and non-positive. There only remains first order equations, i.e. (5.11) if, e.g., the system is indivisible.

One–dimensional Diffusion Equation

Let us study the one-dimensional diffusion equation, (5.6). It is worth while to consider this case in detail, although it lacks some of the features belonging to multi-dimensional spaces.

We assume that D and w are independent of time, and that $D > 0$ everywhere within the system. Suppose that the boundary conditions demand zero current at the boundaries. The equilibrium then corresponds to zero current throughout, or $D(x)a^{0\prime}(x) = w(x)a^0(x)$. We transform to normal coordinates and obtain, with $dz = a^0(x)\,dx$,

$$\dot{\alpha}(z,t) = \frac{\partial}{\partial z}\mathscr{D}(z)\frac{\partial}{\partial z}\alpha(z,t), \tag{5.12}$$

where

$$\mathscr{D}(z) = D(x)(a^0(x))^2, \quad a^0(x) = \exp\{\int^x dx' w(x')/D(x')\}.$$

The term containing w has thus disappeared, and the equation of motion for $\beta(z,t)$ is according to (5.8) given by (5.12), with opposite sign. One may easily verify that the eigenvalues λ_ν are real. Moreover, we have found, in (5.10), that (5.12) tends towards equilibrium.

Show next that (5.12) leads to reversibility in space, in the sense stated in (3.36). The propagator T defined in (3.27) is $T(z_1,t_1;\ z_2,t_2) = T(z_1,z_2,t_1-t_2)$. Therefore the equation of motion

$$\frac{\partial}{\partial\tau}T(z_1,z_2,\tau) = \tfrac{1}{2}\left(\frac{\partial}{\partial z_1}\mathscr{D}(z_1)\frac{\partial}{\partial z_1} + \frac{\partial}{\partial z_2}\mathscr{D}(z_2)\frac{\partial}{\partial z_2}\right)T(z_1,z_2,\tau)$$

is symmetric in z_1 and z_2. Since $T(z_1,z_2,0) = \delta(z_1-z_2)$, one finds macroscopic reversibility in space

$$P_\alpha(z_1\to z_2,\tau) = T(z_2,z_1,\tau) = T(z_1,z_2,\tau) = P_\alpha(z_2\to z_1,\tau). \tag{5.13}$$

Note that (5.13) and the previous conclusions drawn from (5.12) are valid also in the multi-dimensional case if $\vec{w} = 0$ and $D_{ik} = D_{ki}$ in (5.7).

The equation (5.12) is therefore so far in accord with an integral equation with microscopic reversibility in space, $g(z,z') = g(z',z)$. If $g(z,z')$ is asymmetric, eq. (5.12) becomes a less appropriate approximation.

In (5.12) we considered a system with closed boundaries, and therefore the w-term disappeared. If the system instead has periodic boundary conditions, the w-term in (5.6) does remain and is connected with the antisymmetric part of $g(z,z')$. A diffusion approximation to a one-way integral equation is mentioned in § 6, cf. (6.19) and Fig. 3.

Diffusion Approximation

The diffusion approximation is not completely well-defined. Let us indicate one way of deriving its coefficients. We suppose that $G(\vec{x},\vec{x}')$ is given in eq. (2.14), but that the equilibrium need not be known. The assumption belonging to a diffusion approximation is that the kernel G must decrease rapidly when $|\vec{x} - \vec{x}'|$ increases, whereas G varies slowly with change of $|\vec{x} + \vec{x}'|$. We therefore introduce new variables, $\vec{\xi} = (\vec{x} + \vec{x}')/2$ and $\vec{\eta} = \vec{x} - \vec{x}'$, writting $G(\vec{x},\vec{x}') = Q(\vec{\xi},\vec{\eta})$. Since $Q = Q(\vec{x} - \vec{\eta}/2,\vec{\eta})$, we may expand in powers of $\vec{\eta}$ in the former coordinate which varies slowly with $\vec{\xi} = \vec{x} - \vec{\eta}/2$. In the integral equation

$$\dot{a}(\vec{x},t) = \int d^{(m)}\eta\{Q(\vec{x} - \vec{\eta}/2,\vec{\eta})a(\vec{x} - \vec{\eta},t) - Q(\vec{x} - \vec{\eta}/2, -\vec{\eta})a(\vec{x},t)\}$$

we then expand, to second order in η. The result is eq. (5.7) with

$$\left.\begin{aligned} D_{ik}(\vec{x}) &= \tfrac{1}{2}\int d^{(m)}\eta\, G\left(\vec{x} + \frac{\vec{\eta}}{2},\vec{x} - \frac{\vec{\eta}}{2}\right)\eta_i\eta_k \\ \vec{w}(\vec{x}) &= \int d^{(m)}\eta\, G\left(\vec{x} + \frac{\vec{\eta}}{2},\vec{x} - \frac{\vec{\eta}}{2}\right)\vec{\eta}, \text{ where } G(\vec{x}+\vec{\eta}/2,\vec{x}-\vec{\eta}/2) = Q(\vec{x},\vec{\eta}). \end{aligned}\right\} \quad (5.14)$$

The approximation (5.14) appears acceptable, but it usually does not lead to the exact equilibrium distribution, $a^0(\vec{x})$. Thus, consider a one-dimensional integral equation and suppose that $a^0(x) = \text{const.}$ with zero current at the boundaries. If G is symmetric, one does obtain (5.12) from (5.14), but if G is not symmetric there appears a w-term, as implying a non-uniform equilibrium distribution in the diffusion approximation.

§ 6. Examples of Analytic Solutions

This chapter is devoted to exact solutions of the simplest integral equation for continuum variables. The advantages of these examples are threefold. They correspond to typical cases within atomic collisions. They allow solutions of neighbouring equations by perturbation methods. But, foremost, they give a direct insight in the integral equations, showing for instance the similarities and dissimilarities to differential equations.

We consider mainly two extremes. One is symmetric kernels of indivisible systems, as exemplified by multiple scattering at small angles. The other concerns one-way systems, connected with energy loss distributions of energetic particles. Finally, we solve an example of multiple scattering with inclusion of large angles.

Elementary Basic Systems

The simplest kind of continuum systems is the one with displacement invariance in space, cf. eq. (2.6), corresponding to validity of all of the six constraints in § 2. It follows that $g(x,y) = g(x-y)$, and the equilibrium solution is in fact $\alpha^0 = \text{const.}$ for $g = g(|x-y|)$. Note here that we consider primarily the one-dimensional case and, in order to secure simplicity of the analysis, we impose the mild condition of periodicity with an arbitrary long period L. The integral equation is, with $g(\eta)$ real and non-negative

$$\dot{\alpha}(x,t) = \int d\eta g(\eta)\{\alpha(x-\eta,t) - \alpha(x,t)\} \tag{6.1}$$

and that of the conjugate field

$$\dot{\beta}(x,t) = -\int d\eta g(-\eta)\{\beta(x-\eta,t) - \beta(x,t)\}. \tag{6.2}$$

Because of displacement invariance the eigenfunctions of the field are plane waves

$$\alpha_k(x) = \exp(+ikx), \quad \beta_k(x) = \exp(-ikx), \tag{6.3}$$

where $k = 2\pi n/L$. The eigenfunctions obey $\int dx \beta_k(x)\alpha_l(x) = L\cdot\delta_{k,l}$, and $\beta_k = \alpha_{-k}$.

The eigenvalues are, according to (3.15),

$$\lambda(k) = \int d\eta g(\eta)(1 - e^{-ik\eta}). \tag{6.4}$$

Apparently, if $g(\eta)$ is symmetric, i.e. $g(\eta) = g(-\eta)$, the eigenvalues are real and $\lambda(k) = \lambda(-k)$. If there is asymmetry, the eigenvalues are complex

numbers, and $\lambda(k) = \lambda^*(-k)$. The case $k = 0$ corresponds to equilibrium, with $\lambda(0) = 0$. The other eigenvalues have a real part greater than zero.

As to asymptotic behaviour, it is apparent that $g(\eta)$ must decrease faster than $|\eta|^{-1}$ for $|\eta| \to \infty$, in order that the λ_k converge. Similarly, for $|\eta| \to 0$, the symmetric part of $g(\eta)$ must diverge less than $|\eta|^{-3}$, whereas the asymmetric part must diverge slower than $|\eta|^{-2}$. The fundamental solution of (6.1) is the propagator, $T(x,t)$, which for $t = 0$ is $T(x,0) = \delta(x)$. According to (6.1), (6.3) and (6.4) we find for $t \geq 0$,

$$T(x,t) = \frac{1}{L} \sum_k e^{ikx}\, e^{-\lambda(k)t}. \tag{6.5}$$

In the solutions in the following we consider L as infinitely large in (6.4) and (6.5). We replace the summation (6.5) by an integration,

$$T(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx}\, e^{-\lambda(k)t}. \tag{6.5'}$$

The seemingly innocent transition from (6.5) to (6.5′) is not without consequences for the properties of some systems, because the properties depend on the boundary conditions. When (6.5) is applied exactly, the field will return through the periodic boundary, and there will always be an equilibrium $\alpha^0 = 1/L$. If g is asymmetric, the equilibrium has an internal current in the system, and even a one-way system becomes indivisible. If we use (6.5′), however, the field does not return, and the system is an open one. In this case there is uniform equilibrium for a symmetric g, but not for one-way systems. This feature, together with a Galilei transformation of one-way systems, is discussed on p. 39, cf. (6.20). Although one thus finds noteworthy differences between (6.5) and (6.5′), it should be remembered that in practice the solutions of (6.5) and (6.5′) do not differ for finite times t and large L.

The simplest choice of g is the power law

$$g_n(\eta) = \frac{C_n}{|\eta|^{1+n}}. \tag{6.6}$$

We distinguish between the symmetric case

$$g_n^s(\eta) = g_n^s(-\eta) = g_n(\eta), \qquad 0 < n < 2, \tag{6.7}$$

the possible range of n being indicated, and the asymmetric one-way case

$$g_n^a(\eta) = \left\{ \begin{array}{ll} g_n(\eta), & \eta > 0, \\ 0, & \eta < 0, \end{array} \qquad 0 < n < 1. \right\} \tag{6.8}$$

We can now derive $\lambda(k)$, so that it only remains to integrate (6.5′). In the symmetric case we obtain from eqs. (6.6), (6.7) and (6.4)[8]

$$\lambda_n^s(k) = |k|^n \cdot A_n^s, \quad A_n^s = 2C_n \frac{\Gamma(1-n)}{n} \cos\frac{\pi}{2} n = C_n \frac{\pi}{\Gamma(n+1)\sin\frac{\pi}{2} n}, \quad (6.9)$$

where $0 < n < 2$. Correspondingly, in the asymmetric case, from eqs. (6.6), (6.8) and (6.4), for $k > 0$,

$$\lambda_n^a(k) = |k|^n A_n^a, \quad A_n^a = C_n \frac{\Gamma(1-n)}{n} \cdot \exp\left(\frac{i\pi}{2} n\right), \quad (6.10)$$

where $0 < n < 1$, and $\lambda_n^a(-k) = (\lambda_n^a(k))^*$.

The simple structure of solutions for power law kernels may be obtained directly from dimensional arguments. In fact, note that since C_n in eq. (6.6) has the dimensions $x^n t^{-1}$, the corresponding propagators must be of type of $T(x,t) = f_n(x^n/C_n t)x^{-1}$. The semi-group formed by such propagators is thus a stable one[6]. Stable semi-groups are familiar in the mathematical literature, and among the examples to be presented below at least several are well-known in e.g. probability theory[6].

At this point we may illustrate the formulae by an example. Suppose that an energetic ion moves a small distance through a substance, losing a relatively small amount of energy by successive collisions. The distance, or the time elapsed, may represent t in the above equations. The differential cross section times the density of atoms is equivalent to $g(\eta)d\eta$. In the case of multiple scattering g is symmetric, cf. also p. 39. The x-component of the scattering angle in a single collision is $\vartheta_x \propto \eta$, the x-component of the total angle being $\psi_x \propto x$. It is assumed that $\psi_x \langle\langle 1$ and $\vartheta_x \langle\langle 1$. A particle with initial angle 0 has therefore, at time t, the distribution (6.5′). The formulae (6.6) and (6.7) are then power law scattering[15], where Rutherford scattering is the limiting disallowed case at small angles, $n = 2$. In fact, eq. (6.6) corresponds approximately to classical scattering in repulsive power law potentials $\propto R^{-s}$, with $n = 2/s$, so that $1 < s < \infty$ is equivalent to the condition (6.7).

Next, consider the energy loss distribution of the ion. The individual energy loss, η, has a one-sided distribution given by (6.8). The total energy loss, x, is then distributed according to (6.5′). The above power law angular distribution corresponds to $n = 1/s$, so that, again, Rutherford scattering is the upper limit $n = 1$ in (6.8), and $1 < s < \infty$ is the allowed region in (6.8).

Thus, at low angles and for small relative energy losses the power law formula (6.6) serves as a useful basis. In practice, the above formalism without (6.6) has been used in numerical studies of the more complicated case of multiple scattering by Thomas-Fermi type screened Coulomb potentials by Molière[17], cf. also

SCOTT[18] and MEYER[16]. An energy loss distribution was studied by LANDAU[11], in the important but again more complicated case of Rutherford scattering ($n = 1$ in (6.8)) with a cut-off at low energy losses.

Symmetric Distribution, $n = 1$

It is evident that the simplest distributions $T(x,t)$ will result if, in eq. (6.6), n is an integer or a fraction of low order. The symmetric case with $n = 2$, i.e. Rutherford scattering, is divergent, but would have led to a Gaussian distribution in $(x/t^{1/2})$, according to eqs. (6.5′) and (6.9). It is replaced by the second order diffusion equation in § 5. Similarly, the asymmetric case with $n = 1$ is again Rutherford scattering and divergent. In its place appears the first order differential equation in § 5.

For integer n we are left with the symmetric case and $n = 1$. This is apparently multiple scattering with $s = 2$, i.e. closely corresponding to scattering by a repulsive R^{-2}-potential. From eq. (6.9) we get $\lambda_1^s(k) = |k|C_1\pi$, and by integration of eq. (6.5′), for $t > 0$,

$$T_1^s(x,t) = \frac{C_1 t}{x^2 + \pi^2 C_1^2 t^2}. \tag{6.11}$$

This distribution occurs in numerous connections. It is known as the Cauchy distribution[6]. In physical problems it is particularly familiar as a Breit-Wigner formula. The width of the distribution (6.11) increases proportionally to time. If $x \gg \pi C_1 t$, the propagator is $\sim C_1 t x^{-2}$, i.e. determined by a single scattering process from the origin. The system is indivisible with uniform equilibrium, according to eq. (6.1). Correspondingly, we find that, for arbitrary x_1 and x_2, $T(x_1,t)/T(x_2,t) \to 1$ for $t \to \infty$.

We find that eq. (6.11) obeys a second order differential equation of Laplacian type

$$\left(\frac{\partial^2}{\partial x^2} + \frac{1}{\pi^2 C_1^2}\frac{\partial^2}{\partial t^2}\right) T_1^s(x,t) = 0, \qquad t > 0. \tag{6.12}$$

The integral equation in the present case thus picks out one solution of a second order differential equation in time.

It may finally be noted that the propagator corresponding to (6.11) is readily found in a space of dimension $\nu > 1$. The propagator is in fact proportional to $C_1 t \cdot (r^2 + \pi^2 C_1^2 t^2)^{-\frac{\nu+1}{2}}$.

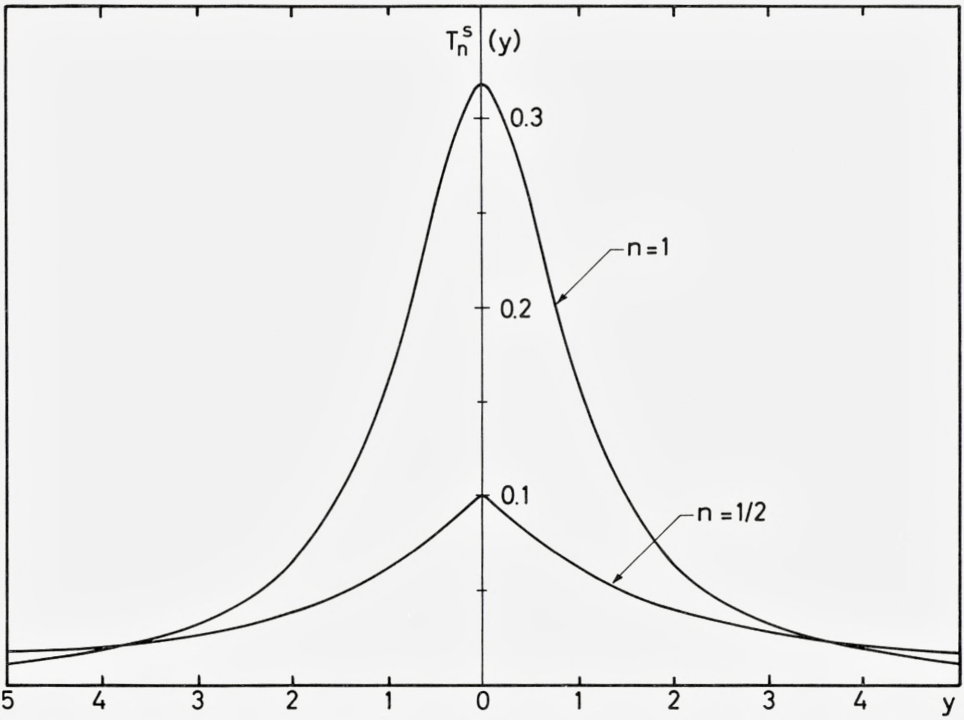

Fig. 1. Symmetric stable distributions for $n = 1$, (6.11), and $n = 1/2$, (6.15), normalized to unity. The abscissa is chosen as $y = x/(C_1 t\pi)$ for $n = 1$, and $y = x/(4C_{\frac{1}{2}}^2 t^2)$ for $n = 1/2$.

One-way Distribution, $n = 1/2$

In the asymmetric one-way case, where $0 < n < 1$, the simplest case must be $n = 1/2$. According to eq. (6.10) one obtains $\lambda_{\frac{1}{2}}^a = |k|^{\frac{1}{2}} C_{\frac{1}{2}} (2\pi)^{\frac{1}{2}} (1 + i)$, $k > 0$. By integration of eq. (6.5′),

$$T_{\frac{1}{2}}^a(x,t) = \frac{C_{\frac{1}{2}} t}{x^{\frac{3}{2}}} \exp\left(- \frac{\pi C_{\frac{1}{2}}^2 t^2}{x} \right), \qquad x \geq 0. \tag{6.13}$$

For large x, the distribution is $\sim C_{\frac{1}{2}} t x^{-\frac{3}{2}}$, and therefore already the first moment, $\langle x \rangle$, diverges. The distribution has a maximum at $x_p = 2\pi C_{\frac{1}{2}}^2 t^2/3$, moving with an acceleration $g = 4\pi C_{\frac{1}{2}}^2/3$. The distribution (6.13) is shown in Fig. 2 together with (6.16).

The propagator (6.13), when considered as an energy loss distribution, as described previously, corresponds to $s = 2$. It thus represents an energy loss distribution associated with the multiple scattering distribution (6.11).

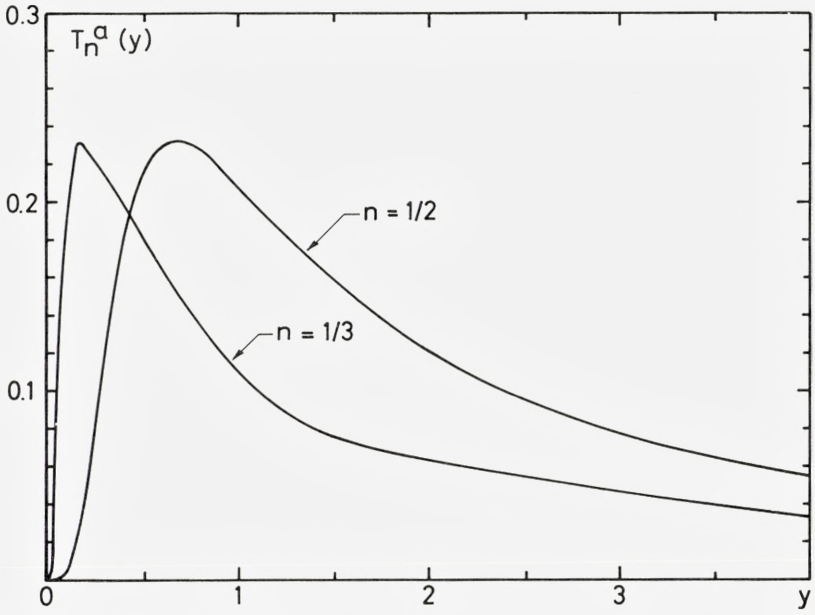

Fig. 2. Stable one-way distributions for $n = 1/2$, (6.13), and $n = 1/3$, (6.16), normalized to unity. The abscissa is chosen as $y = x/(\pi C_{\frac{1}{2}}^{2} t^2)$ for $n = 1/2$, and $y = \text{const} \cdot x/(Ct)^3$ for $n = 1/3$. The scaling for $n = 1/3$ is arbitrarily chosen to give equal heights of the two curves.

Symmetric Distribution, $n = 1/2$

The symmetric distributions are, as it seems, less simple than the asymmetric ones with the same index n. For $n = 1/2$, the symmetric propagator becomes of type of Fresnel's integrals (cf. ref. 1). In fact, the Fresnel g-function is defined as

$$\left.\begin{aligned} g(z) &= \left[\frac{1}{2} - C(z)\right]\cos\left(\frac{\pi z^2}{2}\right) + \left[\frac{1}{2} - S(z)\right]\sin\left(\frac{\pi}{2} z^2\right), \\ C(z) &= \int_0^z \cos\left(\frac{\pi}{2} y^2\right) dy, \qquad S(z) = \int_0^z \sin\left(\frac{\pi}{2} y^2\right) dy. \end{aligned}\right\} \tag{6.14}$$

The g-function is a smoothly decreasing function. It is tabulated in ref. 1; a crude estimate is $g(z) \approx (2 + 4z + \pi^2 z^3)^{-1}$.

The symmetric propagator for $n = 1/2$ becomes, in terms of the Fresnel g-function,

$$T_{\frac{1}{2}}^{s}(x,t) = \frac{2 C_{\frac{1}{2}} t}{|x|^{\frac{3}{2}}}\, g\left\{\frac{2 C_{\frac{1}{2}} t}{|x|^{\frac{1}{2}}}\right\}. \tag{6.15}$$

This function is shown together with eq. (6.11) in Fig. 1. Like eq. (6.11), it tends towards a uniform distribution for $t \to \infty$, and the tails of $T^s_{\frac{1}{2}}$ correspond to single scattering.

One–way Distribution, $n = 1/3$

The index $n = 1/3$ for the asymmetric distribution implies $\lambda^a_{\frac{1}{3}} = |k|^{\frac{1}{3}} \cdot C_{\frac{1}{3}}\, \Gamma(2/3)(3^{\frac{1}{2}} + i)3/2$. The one-third power of $|k|$ indicates connection with Airy functions, and a somewhat lengthy calculation yields in fact, for $x \geq 0$,

$$\left.\begin{aligned} T^a_{\frac{1}{3}}(x,t) &= \frac{Ct}{x^{\frac{4}{3}}} Ai\left(\frac{Ct}{x^{\frac{1}{3}}}\right), \\ C &= C_{\frac{1}{3}}\, 3^{\frac{2}{3}}\, \Gamma(2/3) = C_{\frac{1}{3}}/Ai(0), \end{aligned}\right\} \tag{6.16}$$

$Ai(z)$ being the Airy function[1]. The distribution is shown in Fig. 2. Its general behaviour is somewhat similar to eq. (6.13), but the x-coordinates expand as t^3.

Apart from the above examples a comparatively simple further case is $T^s_{\frac{3}{2}}(x,t)$, which must decrease as $|x|^{-5/2}$ at large $|x|$. It is intimately connected with the so-called Holtsmark distribution[4], but we shall not study it here.

One–way Distribution, n = 1/2, with Screening

The power law scattering (6.6) is a quite special example of displacement invariance. For one, the moments, such as $\langle x^2 \rangle$, are divergent. It is then not easy to compare with a diffusion equation approximation. Next, one-way distributions with finite $\langle x \rangle$ have a constant average velocity, and the corresponding transformation to moving coordinates is of interest. In many practical cases, like energy loss distribution, there will in fact be an upper limit beyond which $g(\eta) = 0$.

Let us therefore briefly study a simple example of screened power law distribution, where $g(\eta)$ in (6.1) is the one-way distribution

$$g(\eta) = \frac{C}{\eta^{\frac{3}{2}}} e^{-\alpha\eta}, \qquad \eta > 0. \tag{6.17}$$

This corresponds to the case (6.8) with $n = 1/2$, as studied above, but now with screening given by the constant α. Transform to dimensionless variables ξ and τ in place of x and t,

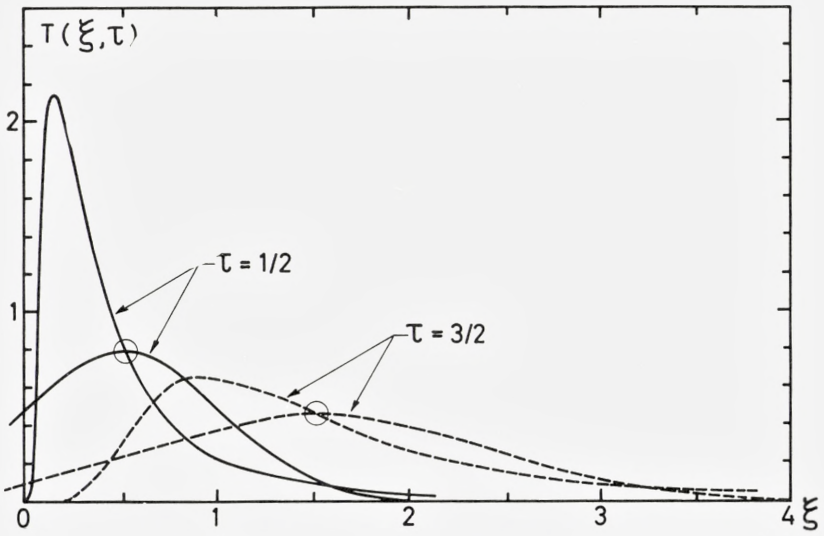

Fig. 3. Screened one-way distribution, (6.18), and its diffusion approximation (6.19), as functions of space, ξ, and time, τ. The asymmetric curves are the exact screened distributions; the symmetric curves represent the diffusion approximation. The two full-drawn curves correspond to time $\tau = 1/2$, and the dashed curves correspond to time $\tau = 3/2$. The exact distribution always intersects the diffusion distribution at its maximum.

$$\xi = x\alpha, \qquad \tau = Ct\cdot(\pi\alpha)^{\frac{1}{2}}.$$

By integration of (6.4) and (6.5′) we get from (6.17)

$$T(\xi,\tau) = \frac{\tau}{\pi^{\frac{1}{2}}\xi^{\frac{3}{2}}} \exp\left\{-\frac{(\tau-\xi)^2}{\xi}\right\}. \tag{6.18}$$

The distribution (6.18) is shown in Fig. 3 for two values of the time variable, $\tau = 1/2$ and $\tau = 3/2$. The average velocity of the distribution is constant, and in fact $\langle\xi\rangle = \tau$. The average square deviation increases with time as $\langle\xi^2\rangle - \langle\xi\rangle^2 = \tau/2$. The most probable point at a given time is $\xi_p(\tau) = -3/4 + (9/16 + \tau^2)^{1/2}$, and is initially accelerated but tends towards having constant velocity, $\xi_p(\tau) \to \tau - 3/4$.

The diffusion approximation (5.14) to the integral equation is determined by the above two moments. The solution of the diffusion equation is a travelling Gaussian distribution,

$$T_{\text{diff}}(\xi,\tau) = \frac{1}{\pi^{\frac{1}{2}}\tau^{\frac{1}{2}}} \exp\left(\frac{-(\xi-\tau)^2}{\tau}\right). \tag{6.19}$$

The diffusion approximation (6.19) is shown together with (6.18) in Fig. 3, for the same values of τ. The deficiencies of T_{diff} are not merely that, for small τ, a substantial part of the function is in the disallowed region $\xi < 0$, but it does not show the skewness of (6.18), for which the maximum ξ_p remains a distance 3/4 behind the maximum of T_{diff}, asymptotically.

Although there is displacement invariance, and $\alpha(x,t) = \text{const.}$ is a solution of eq. (6.1), this is not an equilibrium solution. That is because (6.7) is a one-way system, and $\alpha = \text{const.}$ corresponds to a constant current through the system, which therefore is not isolated. In fact, the ratio $T(\xi_1,\tau)/T(\xi_2,\tau)$ at any two fixed points, $\xi_1 < \xi_2$, tends to zero for $\tau \to \infty$. It is, however, natural to transform to a coordinate system moving with the above constant velocity, i.e. $\xi' = \xi - \tau$. In the ξ'-coordinates the solution $\alpha = \text{const.}$ has no current. We have in fact an isolated indivisible system. In these coordinates both (6.18) and (6.19) tend towards the equilibrium.

The general equation (6.1) can thus be transformed to an isolated rest system

$$\dot{\alpha}(x',t) = \int d\eta g(\eta)\{\alpha(x'-\eta,t) - \alpha(x',t) + \eta \frac{\partial}{\partial x'}\alpha(x',t)\}, \qquad (6.20)$$

provided the velocity $w = \int d\eta g(\eta)\eta$ is convergent. Note that the transformation (6.20) is applicable both for a periodic system and for an open infinite one.

Angular Distribution, $n = 1$

The previous examples of symmetric systems, if applied to multiple scattering, are limited to small angles. Let us show, by means of an example, how the treatment may be extended to large angles. We still suppose that the energy loss of the particle is small within the distances in question. This means that cross sections are time-independent. If v, N and $d\sigma$ are velocity, density of atoms and differential cross section, we can write

$$vNd\sigma = d\Omega S(\vartheta). \qquad (6.21)$$

Here the differential solid angle is $d\Omega = d\varphi d\cos\vartheta$, and ϑ the angle of deflection, while φ is the azimuthal angle. The angular distribution of current is $S(\vartheta)$, depending only on the angle of deflection.

We ask for the propagator $T(\psi,t)$, i.e. the angular distribution at time t, if the angle is $\psi = 0$ at $t = 0$. It obeys the integral equation

$$\left.\begin{aligned} \frac{\partial}{\partial t} T(\psi, t) &= \int_0^{2\pi} d\varphi \int_{-1}^{+1} d(\cos\vartheta) S(\vartheta) \{T(\psi', t) - T(\psi, t)\} \\ &\text{where } \psi' \text{ is given by} \\ \cos\psi' &= \cos\psi\cos\vartheta + \sin\psi\sin\vartheta\sin\varphi. \end{aligned}\right\} \quad (6.22)$$

We expand T in Legendre polynomials, which are the eigenfunctions of the problem. Hereby the integration over φ leads to a factorization, and we obtain finally

$$2\pi T(\psi, t) = \sum_{\nu=0}^{\infty} (\nu + \tfrac{1}{2}) P_\nu(\cos\psi) \exp(-t\lambda_\nu), \quad (6.23)$$

where the eigenvalues λ_ν are

$$\lambda_\nu = 2\pi \int_{-1}^{+1} d(\cos\vartheta) S(\vartheta) \{1 - P_\nu(\cos\vartheta)\}. \quad (6.24)$$

As to $S(\vartheta)$, we ask for an extrapolation of power law distributions (6.6). Let us consider merely the simplest case, corresponding to $n = 1$, and put

$$S(\vartheta) = \frac{C_1 2^{-\frac{5}{2}}}{(1 - \cos\vartheta)^{\frac{3}{2}}}. \quad (6.25)$$

In fact, for $\vartheta \ll 1$, this becomes $S(\vartheta) \to (C_1/2) \cdot \vartheta^3$, where $\vartheta = (\vartheta_x^2 + \vartheta_y^2)^{1/2}$; integrating over ϑ_y we obtain exactly the one-dimensional scattering (6.6) with $n = 1$.

From eqs. (6.25) and (6.24) one gets easily $\lambda_\nu = \pi\nu C_1$ and, finally performing the sum (6.23)

$$T(\psi, t) = \frac{1 - e^{-2\pi C_1 t}}{4\pi[(1 - e^{-\pi C_1 t})^2 + 2e^{-\pi C_1 t}(1 - \cos\psi)]^{3/2}}. \quad (6.26)$$

When $C_1 t \ll 1$, the main part of $T(\psi, t)$ is within small angles, and $T \approx (C_1 t/2)(\pi^2 C_1^2 t^2 + \psi^2)^{-3/2}$, i.e. it becomes the two-dimensional version of eq. (6.11). For large values of t, the distribution (6.26) tends to the uniform distribution, in agreement with eq. (6.22) being an indivisible system, with equilibrium $T = (4\pi)^{-1}$.

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