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ON THE THEORY OF MEASUREMENT AND ITS CONSEQUENCES IN STATISTICAL DYNAMICS

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CONTENTS

Synopsis

It is attempted to analyse questions of probability common to statistical physics, mathematical statistics, and measurements. Idealized measurements may be used as a starting-point and general irreversible equations of motion of a field as an aid in the analysis. When a field remains independent of a measurement, the measurement contains a simple statement about the field. It is found that the statement is in terms of, not an absolute entropy, but a relative entropy measuring the field with respect to observed frequencies, or in terms of other relative degradation functions. This central question is elucidated further by irreversible equations of motion, showing that only relative entropy, or degradation functions, have the necessary monotonic behaviour. The frequent use of absolute entropy in various disciplines is commented upon. It is found, however, that a new absolute function of the field exists for time-independent equations of motion. Fields dependent on the measurement are also analysed. It is shown how an effective time reversibility in equilibrium may result from irreversible equations of motion.

It turns out to be necessary to look into a celebrated issue in mathematical statistics. This is done separately in § 5, where it is shown how probability statements of outcome of measurements may be inverted to statements about the field from given experimental results. The discussion concerns discrete variables and one-way continuum variables.

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§ 1. Introduction

I should begin by forewarning the reader. I am to be concerned with measurements in physics, but will be in danger of conjuring up mathematical fictions rather than events of the real world, since the measurements are conceived in terms of probabilistic Gedankenexperimente. However this may be, the main purpose of the study of measurements is to obtain a stepping stone to fundamental concepts and methods in the dynamics of physical systems.

The present paper has, apparently, a simple pattern. The introduction is mainly concerned with a classification of fields and measurements, and the equations of motion are mentioned briefly. One class of measurements is that where the field remains independent of a measurement, as treated in § 2. At first I discuss direct measurements of an independent field, a subject connected with familiar mathematical statistical methods, like the simple theory of errors. Next, from the measurements one may want to determine the independent field at earlier and later times, and we shall look into the interesting difference between the two cases. Above all, measurements of independent fields lead directly to degradation functions, like entropy, as measures of probability, but in a more general sense than usually conceived. In fact, as shown in § 3, functions like entropy are not absolute measures of a probability field but only relative measures of one field with respect to another one. One absolute function of the field does exist, however, if the equations of motion are time-independent. In the second class of measurements the field depends on the measurement, as discussed in § 4. For successive measurements the properties of Markov chains are obtained in the simpler cases. Dependent fields give possibility of analyzing a basic situation in statistical mechanics, and it is shown how irreversible equations of motion can result in time reversibility in equilibrium.

The first subject mentioned above, i.e. the familiar direct measurement based on the theory of errors or similar statistical methods, turns out to contain unsuspected and treacherous pitfalls. This is because probability statements in measurements are not the desired ones about the unknown field. Such problems are well-known in mathematical statistics but mainly ignored in physics; they have led to a schism connected with a celebrated suggestion by BAYES. It is necessary, therefore, to look into the probability content of basic measurements. In order not to confuse the main issue of this paper, I have stated the relevant results briefly in § 2. The detailed analysis is postponed to § 5, where it is shown how measurements can yield probability statements as regards the parameters in the theory.

It might be asked why one should discuss, in such detail, abstract measurements as well as an abstract theory, with emphasis laid on probability and irreversibility. A general reason — already inherent in the question — is that probability in physics, primarily in statistical mechanics but also in quantum mechanics, gives rise to much more serious and profound problems than often envisaged. I need not remind of the remarkable differences in point of view in BOLTZMANN's and GIBBS' treatments of statistical mechanics, of the discussions between EINSTEIN and BOHR on quantum theory, or of the more recent information theory approach where the existence of an absolute entropy is claimed before the laws of physics are invoked. It should be emphasized, however, that any measurement is intimately connected with probability and constitutes by itself an irreversible process. On the one hand, if one wants to analyse the basic interpretation of quantum theory it is particularly important to account consistently for probability concepts and for irreversibility. On the other hand, for practical purposes it is useful to formulate a simple general theory, even though it necessitates somewhat abstract concepts. I am well aware that these remarks are somewhat scattered, and that the following discussion too consists of scattered solutions of the major problems aimed at.

Terminology and equations of motion

It might be useful, before completing the introductory discussion, to explain some basic concepts and terminology connected with the equations of motion of the field. The term 'statistical dynamics' is meant to indicate that there is an arrow on the time variable in the equations of motion, and that a field usually has conservation and is non-negative. The general description is discussed in detail in a previous paper[12], in the following referred to as SSD. I do not invoke the Hamiltonian equations of motion but use a more general formulation where irreversibility is explicit. If so desired, the reader may consider it as retarded solutions of the equations of motion, as exemplified by Brownian motion of a Hamiltonian system.

We are concerned with a coordinate variable, which may be discrete ($j = 1,2,3,\ldots n$), or continuous. Consider, for definiteness, a discrete variable and introduce an initial field $\bar{A} = (A_1, A_2, A_3, \ldots, A_n)$ where $A_j \geq 0$ and $\sum_j A_j = 1$. In a linear theory, a final field $\bar{a} = (a_1, a_2, a_3, \ldots, a_n)$ is then determined by $\bar{A}$ and by transition rates T_{kj} from state j to state k by

$$\bar{a} = \bar{\bar{T}} \cdot \bar{A}, \text{ or } a_k = \sum_j T_{kj} A_j, \tag{1.1}$$

where we must assume $T_{kj} \geq 0$ in order that $a_k \geq 0$, and $\sum_k T_{kj} = 1$, so that $\sum_k a_k = 1$.

The propagator $\bar{\bar{T}}$ should be considered as resulting from equations of motion of type of

$$\frac{\partial}{\partial t} a_k(t) = \sum_j \{G_{kj}(t) a_j(t) - G_{jk}(t) a_k(t)\}, \tag{1.2}$$

where $G_{kj}(t) \geq 0$. In (1.1) the fields $\bar{A}$ and $\bar{a}$ can then be, respectively, $\bar{a}(t')$ and $\bar{a}(t'')$, $t'' \geq t'$, so that $T_{kj} = T_{kj}(t'',t')$. In the case of continuum variables the above equations remain valid if $j \to x'$, $k \to x''$, so that e.g., $T = T(x'',t'';x',t')$ and $a_k(t) \to a(x,t)$. If the coefficients G in (1.2) are time-independent, the propagator is a function of the time difference only, $T = T(x'',x',t''-t')$, and there is a unique equilibrium for indivisible systems (cf. SSD). A main point is that $T(x'',t'';x',t')$ does not exist for $t'' < t'$, and for discrete variables the propagator T_{kj} does not fulfill the rule of non-negative fields when $t'' < t'$.

Note that the variable t need not be time, so that any one-way variable will do as well. One example is the path length moved by a particle suffering collisions and being possibly slowed down. Transformations between one-way variables are exhibited in § 5.

Measurements and interpretation of fields

Measurements are irreversible processes. I shall not here investigate this basic aspect of measurements but only note that it is not at variance with the above-mentioned irreversible equations of motion. The problem with which we shall be concerned is the probability property of measurements. In fact, in the following it will be supposed that a measurement is a more or less imperfect sampling, in the sense of mathematical statistics. Though plausible, also this assumption would seem to require an explanation, concerning its consistency and its connection to the theory of physics. I refrain from a closer discussion but, in part, the consistency will be elucidated.

It is useful to make a classification of measurements, and of the field to be measured. First, one may want to find from a measurement the immediate value of the field, $\bar{a}(t)$. This is clearly the simplest case, and there is also little difficulty in finding from it the field at a later time. Second, in many physical problems one asks preferably for a previous field $\bar{a}(t-\tau)$, as introduced above. One is here up against the difficulty that, whereas $\bar{a}(t)$ may be determined from $\bar{a}(t-\tau)$ according to (1.1), the inverse determination of $\bar{a}(t-\tau)$ is not straightforward, mainly because a propagator backwards in time does not exist. There is thus no symmetry between past and future, and it becomes more difficult to predict the past than the future.

As to the interpretation of the field, $\bar{a} = \bar{a}(t)$, and its relation to measurements, one may meet with several situations. We confine the discussion to two major cases. In these classifications I distinguish between properties of the measurements and properties of the field. The distinction is convenient but not strictly correct. In the end, most of the properties of the field, like its independence, are determined by the measurement and by the parameters one decides to measure.

Independent field

In one type of field measurement the field remains independent of the measurement. A familiar phenomenon of this kind is an incoming current of identical, but independent, particles, which suffer collisions in a gas. The incoming current is supposed to have a steady probability distribution in space and in momentum. One measures each time on a new particle, but on the same probability distribution. A similar example of independent fields is observations of the spectral distribution of electromagnetic radiation from a star.

One may perform measurements at various time instances and collect information about the field. By time is meant the independent one-way variable of the field, e.g., the path length moved or the time variable for each particle. The spatial variable of the field can be coordinate space, momentum space, or phase space; and it may alternatively be considered as a discrete variable, for instance when counters are used. Each measurement concerns a new particle whose behaviour is independent of the others but governed by the same field $a(x,t)$. The theory of independent fields is discussed in § 2.

Dependent field

In the second case the field depends on the measurement. Consider the above-mentioned current of particles through a gas, or a Brownian motion. One may measure the generalized coordinates of a particle at a certain time, and ask for the new probability distribution of it at subsequent and even at prior times. This case is to be discussed in some detail. However, this case may also be conceived in a more general way. The 'particle' may be a small or large physical system and its distribution is then the ensemble of Gibbs, but now governed by explicitly irreversible equations of motion. From a mathematical point of view the measurements of dependent fields can have connections to Markov processes, as we shall see. Measurements of a dependent field may alternatively be considered as preparations of a system in a more or less well-defined state. But it should be remembered that the basic preparation of systems, before performing experiments, is to let them achieve equilibrium, whereby a quite definite state is obtained with comparative ease. The dependent field is treated in § 4.

The above division into classes of fields and measurements appears to be useful. Still, in actual measurements one may be concerned with, say, a mixture of independent and dependent fields. Thus, in measurements of Brownian motion, SVEDBERG observed the number of particles in a small volume at successive time instances. For particles which enter the volume one is concerned with the independent field, while for those which have been observed it is the dependent field.

Usually, the field is normalized to unity or to a certain particle number, and so is the measurement. This holds particularly for the case of dependent fields. But often the field or the measurement does not represent a fixed number of particles. Fields of this kind correspond to the grand ensemble of Gibbs, with particular mathematical simplifications. Measurements without a fixed number of particles are familiar in the form of Poisson distributions.

§ 2. Measurements of Independent Fields

The concept of measurement of independent fields was explained in the introduction. In some respects this case is the simplest one. In fact, when the field is independent one may perform an arbitrary number of measurements of the same field, and none of the results will be influenced by any of the others. I consider primarily the simpler case of measurement of the immediate field $\bar{a}$, but will take up measurements of previous and later fields at the end of this chapter.

Probability by measurement of immediate field

Direct measurements of an independent field are closely connected to a subject treated extensively in textbooks on statistical methods and probability. Furthermore, if one is concerned with a large number of recordings there is little difficulty in interpreting the results in a straight-forward way. Yet, the simple measurements contain a celebrated problem and other difficulties which have to be discussed and clarified, because of their importance to measurements in physics. These difficulties arise since a normal statistical statement gives only the probabilities of various outcomes, assuming the parameters (the field $\bar{a}$) to be known. In a measurement, on the contrary, one wants a statement, possibily a probability statement, as regards the unknown parameters for a given outcome. I call this the question of inversion of probability. The question was raised by BAYES in 1763[1] but even in present mathematical statistics there are several schools of thought about it.

In order not to confuse the main issue of the present paper, I now give merely a summary discussion of the direct measurement, with preliminary statements as to the inversion of probability. A more detailed analysis is necessary but it is postponed to § 5, at the end of the paper.

The discussion of measurements is rather different for fields, a_k, depending on a discrete coordinate variable, and fields $a(x)$ with a continuum variable. For the present I confine the discussion to discrete variables, where the number of unknown quantities to be determined is explicitly finite. The field is $\bar{a} = (a_1, a_2, \ldots, a_n)$, $\sum a_i = 1$, and thus any function, f_i, depending on the discrete variable i has a value (average) $\langle f \rangle = \sum f_i \cdot a_i$.

The elementary measurement is taken to be a single count in one of the n places. To the i'th outcome is ascribed a probability, assumed to be given by the number a_i. Let N elementary measurements be performed. The basic assumptions are that the measurements are independent and indistinguishable. From independence it follows, first, that all measurements have the same probability field $\bar{a}$ and, second, that the probability of a composite event is the product of the individual probabilities. It is thus possible to assign a probability to every set of measurements. The assumption of indistinguishable measurements is merely a simplification, implying that any ordering of the events is immaterial and that only the total number of recordings, N_i, in each of the n places is of significance. Thus, it follows that the result of N measurements* is completely specified by $\overline{N} = (N_1, N_2, \ldots, N_n)$, where $N_i = 0,1,2, \ldots$ and $\sum N_i = N$.

From the above it can be concluded that the probability of $\overline{N}$, for given $\bar{a}$ and N, is the familiar formula

$$P_{\bar{a},N}(\overline{N}) = \frac{N!}{N_1! N_2! \ldots N_n!} a_1^{N_1} a_2^{N_2} \ldots a_n^{N_n}. \tag{2.1}$$

Again, a function $f(\overline{N})$ has a value given by $\langle f \rangle = \sum_{\overline{N}} f(\overline{N}) P_{\bar{a},N}(\overline{N})$, the summation being over all $\overline{N}$ belonging to N. In particular, it is observed that (2.1) implies $\langle N_i/N \rangle = a_i$. The main significance of (2.1) is the rules of probability contained in it. In addition to the discussion above, it may be mentioned that (2.1) obeys the rule of additivity of probabilities. Thus, (2.1)

* Note that the distinction between a single measurement and N measurements is usually a convention. The N measurements may be conceived as, and may actually be, a single measurement, i.e. one N-measurement.

is one of the terms in $(a_1 + a_2 + \ldots + a_n)^N = 1^N$, and here one can join elements, $a_{12} = a_1 + a_2$, if the counts are joined, $N_{12} = N_1 + N_2$.

These remarks are meant to illustrate the uniquely defined properties of probabilities for outcome of measurements. The main features are those of mass distributions. It is not necessary to invoke a connection between probabilities and frequencies belonging to real measurements. Instead, in the mathematical limit of $N \to \infty$ the numbers N_i/N converge towards a_i, since according to (2.1) $\langle (N_i/N)^s \rangle \to a_i^s$, for $s \geq 0$.

The measurement described by (2.1) concerns a fixed number of counts, N. It is often convenient to relax this bond. Calculations can be simpler if the N_i are completely independent. In fact, many physical measurements are just of this kind. Thus, one may have n identical counters measuring intensities of a scattered beam. The intensities are proportional to a_i. If all counters are open during the same time interval, the individual countings are independent and have probabilities $p_{a_j,M}(N_j)$, where

$$p_{a_j,M}(N_j) = \frac{(Ma_j)^{N_j}}{N_j!} e^{-Ma_j}, \quad j = 1,2,\ldots,n. \tag{2.2}$$

The probabilities (2.2) are the familiar Poisson distributions. The total probability is

$$P_{\bar{a},M}(\bar{N}) = \prod_{j=1}^{n} p_{a_j,M}(N_j) = e^{-M} \prod_{j=1}^{n} \frac{(Ma_j)^{N_j}}{N_j!}, \tag{2.3}$$

which formula is not unlike (2.1). The parameter M is also the total average number of counts, $M = \sum_j \langle N_j \rangle$, and it is proportional to the time during which the counters are open. The measurements (2.1) and (2.2) are analogous to the statistical mechanical concepts of petit ensembles and grand ensembles, respectively.

Distribution of immediate field from measurement

I now turn to the actual problem of inversion of probability, i.e. the possibility of a probability statement as regards $\bar{a}$ for a given observation $\bar{N}$. It should be emphasized from the start that the experiment stated in (2.1) does not—when unmodified—allow of unique inversion of probability. In § 5 it will be shown how a slight modification leads to inversion of probability, and also how inversion obtains in the continuum case without modification of the experiment. The aim here is merely to quote from § 5 the results as regards inversion of probability, for a discrete variable. Still, it seems appropriate to accompany the formulae by qualitative arguments which, I hope, make the results plausible. In addition, such arguments emphasize that, for large N_i, there is little difference between the various points of view on inversion.

Suppose for simplicity that $n = 2$ in (2.1), so that there is only one parameter, a_1, since $a_2 = 1 - a_1$. In the limit of large N, the formula (2.1) then becomes

$$P_{a_1, N}(N_1) \propto \exp\left\{-\left(\frac{N_1}{N} - a_1\right)^2 \Big/ 2\sigma^2\right\},$$

where $\sigma^2 \sim a_1 (1 - a_1)/N \sim (N_1/N)(1 - N_1/N)/N$ may be considered as a constant. If N_1/N is taken to be a continuum variable, the distribution is Gaussian in the variable $a_1 - N_1/N$, and thus the unknown parameter a_1 has a Gaussian distribution about N_1/N.

Because of the above asymptotic results, the direct probability (2.1) will in some respects correspond to a probability of $\bar{a}$ for given $\bar{N}$. Introduce therefore a factor taking account of this contribution,

$$L_{\bar{N}}(\bar{a}) = a_1^{N_1} a_2^{N_2} \ldots . a_n^{N_n} = \exp\left(\sum_{i=1}^{n} N_i \log a_i\right). \tag{2.4}$$

The quantity L in (2.4) is often called likelihood, a term introduced by R. A. FISHER[8]), in order to emphasize that one is not concerned with a probability. But in contrast to the original notion of FISHER, the likelihood is here part of a distribution of the field $\bar{a}$.

The differential distribution af $\bar{a}$ may be written on the form, cf. (5.22),

$$\tilde{P}_{\bar{N}}(\bar{a}) \cdot \frac{da_1}{a_1} \cdot \frac{da_2}{a_2} \cdot \ldots \cdot \frac{da_n}{a_n} \cdot \delta\left(\sum_i a_i - 1\right), \tag{2.5}$$

where the δ-function takes care of the bond between the values of a_i. The integral of (2.5) over all values of a_i ($0 \leq a_i \leq 1$) is normalized to unity.

Write next $\tilde{P}$ as

$$\tilde{P}_{\bar{N}}(\bar{a}) = C \cdot L_{\bar{N}}(\bar{a}) \cdot w(\bar{a}), \tag{2.6}$$

where $w(\bar{a})$ is an uncertainty factor and C accounts for normalization.

The distribution $\tilde{P}_{\bar{N}}(\bar{a})$ is bracketed within a relatively narrow interval of probability distributions. This is expressed by the uncertainty factor $w(\bar{a})$ in the following way

$$
\left.\begin{aligned}
w(\bar{a}) &= a_1^{\xi_1} a_2^{\xi_2} \ldots\ldots a_n^{\xi_n}, \\
\text{where} \\
\sum_{i=1}^{n} \xi_i &= 1,\ 0 < \xi_i < 1.
\end{aligned}\right\} \tag{2.7}
$$

The value of the normalization constant C in (2.6) is seen to be

$$C(\bar{N}+\bar{\xi}) = \frac{\Gamma(N + \sum \xi_i)}{\Gamma(N_1+\xi_1)\Gamma(N_2+\xi_2)\ \ldots\ \Gamma(N_n+\xi_n)}. \tag{2.8}$$

The factor w thus represents an uncertainty in the probability, but the uncertainty is usually quite negligible. Its magnitude can be ascertained in the estimate of any average by varying $\bar{\xi}$ in (2.7).

Note that the distribution $\tilde{P}_N(\bar{a})$, according to (2.4), (2.5), (2.6), and (2.7), obeys the same rule of composition as (2.1). Thus, if a_1 and a_2 are combined to one variable, $a_{12} = a_1 + a_2$, by integrating away one variable in (2.5), then one obtains again the same formulae with one variable less and $N_{12} = N_1 + N_2$, as it should be.

In the following I make use of the likelihood (2.4) with $C = C(\bar{N})$ as a sufficiently well-defined representation of inverse probability, the small uncertainty in w being tacitly understood.

Degradation functions and accuracy of field

The likelihood represents approximately the probability of a field $\bar{a}$ for a given measurement $\bar{N}$, when N is large. It may be reformulated in the following way. Let $\bar{\nu} = (\nu_1, \nu_2, \ldots \nu_n)$, such that $\sum_i \nu_i = 1$, introduce a quantity $S_{\bar{\nu}}(\bar{a}')$ by

$$S_{\bar{\nu}}(\bar{a}') = \sum_{j=1}^{n} \nu_j \log \frac{a_j'}{\nu_j} \leq 0, \tag{2.9}$$

and call it the relative entropy of $\bar{a}'$ with respect to $\bar{\nu}$. The relative entropy is equal to zero only when $a_j' = \nu_j$ for all j, i.e. $\bar{a}' = \bar{\nu}$. If we introduce $\nu_i = N_i/N$, and disregard the uncertainty factor w, we can express the distribution (2.5), (2.6) in terms of the likelihood

$$\tilde{P}_{\bar{N}}(\bar{a}') \cong C(\bar{N}) L_{\bar{N}}(\bar{a}') \cong \exp(N S_{\bar{\nu}}(\bar{a}')). \tag{2.10}$$

When N is large one finds that (2.1), from STIRLING's formula, is also represented by (2.10). It is obvious that, when N becomes large, the field $\bar{a}$

and the measured frequency $\bar{\nu}$ deviate less and less from one another. In this limit we may expand in (2.9), assuming $\bar{\nu} \approx \bar{a}$, and find

$$S_{\bar{\nu}}(\bar{a}') \cong -\sum_j \frac{(a_j' - \nu_j)^2}{2\nu_j} = -\sum_j \frac{a_j'^2}{2\nu_j} + \frac{1}{2} \cong -4(1 - \sum_j (a_j'\nu_j)^{1/2}). \tag{2.11}$$

The above formulae may be used to find how closely an N-measurement determines a field. To this end suppose that the field is $\bar{a}$. We make an N-measurement with outcome $\bar{N}$, and obtain a normalized likelihood $\tilde{P}_{\bar{N}}(\bar{a}') = C(\bar{N}) \cdot L_{\bar{N}}(\bar{a}')$ for the field being $\bar{a}'$. If we average over all possible outcomes N_i, with normalized probability (2.1) and $\sum_i N_i = N$, we find the probability of $\bar{a}'$, for a given $\bar{a}$. Thus

$$\left.\begin{aligned} \tilde{P}_{\bar{a}}(\bar{a}') = \sum_{N_1, N_2 \ldots} \frac{N!}{N_1! \ldots\ldots N_n!} \frac{(N-1)!}{(N_1-1)! \ldots\ldots (N_n-1)!} \\ \cdot (a_1 a_1')^{N_1} \ldots\ldots (a_n a_n')^{N_n}. \end{aligned}\right\} \tag{2.12}$$

Introduce here STIRLING's formula in the form $N! \cong (2\pi N)^{1/2} N^N e^{-N}$, and neglect small terms which are in fact of order of magnitude of the uncertainty in w.

The important thing to notice is that (2.12) is symmetric in $\bar{a}$ and $\bar{a}'$, and since only one degradation function, (3.4), is symmetric in the variables we should use that, i.e.

$$D_{\bar{a}}^{(-1/2)}(\bar{a}') = \sum_i (a_i a_i')^{1/2}. \tag{2.13}$$

In fact, introduce in (2.12) the quantity $\alpha_j = (a_j a_j')^{1/2}/(\sum_k (a_k a_k')^{1/2})$, where $\sum_j \alpha_j = 1$, and find

$$\tilde{P}_{\bar{a}}(\bar{a}') \cong \sum_{N_j} (2\pi)^{-n+1} \prod_i \left(\frac{N\alpha_i}{N_i}\right)^{2N_i} \cdot (D_{\bar{a}}^{(-1/2)}(\bar{a}'))^{2N},$$

or, replacing the summations by integrations over $\nu_i = N_i/N$,

$$\left.\begin{aligned} \tilde{P}_{\bar{a}}(\bar{a}') \cong (D_{\bar{a}}^{(-1/2)}(\bar{a}'))^{2N} \cong \exp\{-2N(1 - D_{\bar{a}}^{(-1/2)}(\bar{a}'))\} \\ = \exp\{-N\sum_i (a_i^{1/2} - a_i'^{1/2})^2\}. \end{aligned}\right\} \tag{2.14}$$

It is not surprising that (2.14) is essentially the square root of (2.10) if a_i is replaced by ν_i. Eq. (2.14) was derived on the assumption that N is large. But in this limit a_i' is close to a_i, and then the uncertainty implied by $w(\bar{a}')$ in (2.7) becomes quite small. Therefore, (2.14) closely represents a probability and the small uncertainty may be estimated. One may thus use (2.14) to find how large N has to be in order that a given accuracy obtains.

If a Poisson measurement (2.2) were used instead of the N-measurement, the calculation would be slightly simplified. Still, the main result, i.e. the appearance of $D^{(-1/2)}$, comes about in a surprisingly simple way in the above derivation of (2.14).

From the result (2.14) it may be concluded that degradation functions like (2.13) should tend monotonically to unity with time. Thus, suppose that one chooses to make an N-measurement, with a very large value of N, in order to be able to distinguish between two fields $\bar{a}$ and $\bar{a}'$. Let the fields obey the equation of motion (1.2). Such equations of motion contain a smearing of the fields so that with increasing time it should become less easy to distinguish between them. One expects therefore that an N-measurement gives inferior distinction if performed at a later time instant. But this means that $D^{(-1/2)}$ in (2.13) always tends towards unity. In fact, this monotonic behaviour is proven generally in § 3, cf. (3.13).

Independent field before and after measurement

In this section it is still assumed that an N-measurement is performed at time t. With given equations of motion one asks for statements as to the fields at earlier and later times, to be called respectively the previous and the later fields.

Consider the simple case of the later field. Let the field at time t, $\bar{a}(t)$, have a given distribution, e.g., (2.5). The later field, $\bar{a}(t+\tau)$ with $\tau > 0$, is easily obtained, because it is uniquely given by the propagator of the equations of motion, (1.1), $\bar{a}(t+\tau) = \bar{\bar{T}}(t+\tau,\ t) \cdot \bar{a}(t)$. Indeed, the estimate of the value of any function $f(\bar{a}(t+\tau))$ is obtained as an average over (2.5), i.e. $\langle f(\bar{\bar{T}}(t+\tau,t)\cdot \bar{a}(t))\rangle$.

Quite apart from such results, the mere fact that $t+\tau$ is later than t reduces the freedom of choice of $\bar{a}(t+\tau)$. Consider thus the two differential volume elements $d^{(n)}a(t) = da_1(t)\cdot da_2(t) \ldots . da_n(t)$ and its time transform $d^{(n)}a(t+\tau)$. Because of the linear equations of motion their connection is established directly. Note that the δ-function in (2.5) may be left out because it is conserved, the sum $\sum a_i$ being a constant of the motion. From (1.1) the volume elements are found to be connected by the determinant of the propagator matrix,

$$d^{(n)}a(t+\tau) = |\bar{\bar{T}}(t+\tau,t)|\, d^{(n)}a(t), \qquad (2.15)$$

where it is readily shown that

$$|\,\bar{\bar{T}}(t+\tau,t)\,| = \exp\left\{-\sum_{k+j}^{n}\int_{t}^{t+\tau} G_{kj}(t')\,dt'\right\}. \tag{2.16}$$

For time-independent equations of motion the determinant (2.16) decreases exponentially with τ,

$$|\,\bar{\bar{T}}(t+\tau,t)\,| = \exp\left\{-\tau\sum_{s=0}^{n-1}\lambda_s\right\}, \tag{2.16'}$$

λ_s being the eigenvalues of the equation of motion, cf. SSD.

It follows that the available volume in $\bar{a}$-space shrinks with time, decreasing exponentially according to (2.16′) and exceedingly fast when n is large. Moreover, the equation (2.16′) indirectly expresses the fact that, whatever the initial field $\bar{a}(t)$, the later field for large τ must approach the equilibrium field $\bar{a}^0$.

More delicate problems arise in connection with determination—from a measurement at time t—of a previous field, $\bar{a}(t-\tau)$, where therefore $\bar{a}(t) = \bar{\bar{T}}(t,t-\tau)\,\bar{a}(t-\tau)$. One difficulty is that the inverse propagator does not exist, as is more obvious in the continuum case. In the discrete case, the equations (2.15) and (2.16′) make it clear that if the field did exist at time $t-\tau$, the measured field at time t has a strongly confined region of permissible values.

Another difficulty is that the field at time t is itself influenced by the previous existence of the field. In the extreme case where the field is known to exist at time $-\infty$, the field at t must be the equilibrium field $\bar{a}^0$, and it would be futile to attempt a measurement, unless the equilibrium is unknown. Suppose instead that the field is known to exist at time $t-\tau$. In attempting to find $\bar{a}(t)$ one should in (2.5) express this field in terms of the unknown $\bar{a}(t-\tau)$, the differential volume element being given by (2.15). Therefore (2.5) becomes

$$\left.\begin{aligned}&\tilde{P}_N(\bar{\bar{T}}(t,t-\tau)\cdot\bar{a}(t-\tau))\cdot|\,\bar{\bar{T}}(t,t-\tau)\,|\,d^{(n)}a(t-\tau)\cdot\\ &\cdot\,\delta(\sum_i a_i(t-\tau)-1)\cdot\prod_{j=1}^{n}\{\sum_l T_{jl}(t,t-\tau)\cdot a_l(t-\tau)\}^{-1},\end{aligned}\right\} \tag{2.17}$$

stating indirectly the distribution of $\bar{a}(t)$.

As to the determination of the field at earlier times, the distribution of the field at $t-\tau$ is given directly by (2.17), unless it is known to exist before $t-\tau$. Look apart from the latter subtlety and suppose also that N is large so that the likelihood (2.4) gives the dominating probability factor. The probability for $\bar{a}(t-\tau)$ is then essentially given by (2.10), i.e.

$$C(\bar{N}) \cdot L_{\bar{N}}(\bar{\bar{T}} \cdot \bar{a}(t-\tau)) \cong \exp\left\{N \sum_{j=1}^{n} \nu_j \log \frac{\sum_{k=1}^{n} T_{jk}(t, t-\tau) a_k(t-\tau)}{\nu_j}\right\}, \quad (2.18)$$

where $\nu_j = N_j/N$.

These brief remarks were meant to indicate the problems connected with previous fields, when the fields are independent. But such cases are quite common in practical measurements, and ad hoc procedures are often used for their solution. A basic property of $\bar{a}(t-\tau)$ is that its components are non-negative, and any prescription which takes account of this can give quite good estimates.

For dependent fields, the corresponding questions of earlier and later times have somewhat different implications, as discussed in § 4.

§ 3. The Relative Degradation Functions and Their Change with Time

It seems proper to indicate a few of the reasons why it may be rewarding to undertake the following, somewhat lengthy, study of relative degradation functions (cf. SSD) and their time behaviour.

First, we have already seen that several of the degradation functions come into play if we make a measurement and ask for the probability of a field, or if we want to distinguish between two fields by a measurement. The degradation functions in question were relative in the sense that they measured one field with respect to another one. Now, we were also concerned with the change in time of fields, where the irreversible equations of motion must lead to a smearing of fields, so that in some sense they approach each other. The quantitative expression for such a tendency, if it has a meaning at all, should apparently be sought for in the degradation functions. Again, the tendency should not depend on the existence of an equilibrium distribution or on time-independence of the equations of motion.

Second, in statistical mechanics the function entropy is used extensively and connected to absolute probabilities. In the theory of information the entropy is often claimed to be a unique measure of information, and this has been used as a basis for an alternative approach to statistical mechanics. It seems important to investigate such claims, and to look into the role of the other degradation functions since they have the same general properties as entropy. To this end, the time behaviour of the functions will be studied on the basis of quite general equations of motion.

It turns out, above all, that neither the entropy nor the other degradation functions have consistent meaning if regarded as absolute functions; they are relative functions measuring one dynamic field with respect to another one. The reader may also notice that the preceding discussion of measurements, albeit idealized ones, led to relative degradation functions only.

Degradation functions

I now attempt a precise discussion of the degradation functions. This family of functions was derived in SSD. They are averages of functions depending on the field a, with the property of separability for independent systems. In SSD we considered only degradation functions for the equilibrium field with respect to a time-dependent field. Since I now drop the assumption of time-independent equations of motion, an equilibrium field does not necessarily exist. Consider continuum variables—discrete variables being a special case of this—and introduce the relative degradation function of n'th order for the field $a_2(x,t)$ with respect to $a_1(x,t)$,

$$D^{(n)}_{a_1(x,t)}(a_2(x,t)) = \int dx\, a_1(x,t)\left(\frac{a_1(x,t)}{a_2(x,t)}\right)^n, \quad -\infty < n < \infty, \tag{3.1}$$

where the integration extends over the total volume, and where, as indicated, n is any number on the real axis. The functions a_1 and a_2 are positive and

$$\int a_1(x,t)\,dx = \int a_2(x,t)\,dx = 1. \tag{3.2}$$

It may be noted that

$$D^{(n)}_{a_1}(a_2) = D^{(-1-n)}_{a_2}(a_1), \tag{3.3}$$

and, in particular, the only symmetric function is

$$D^{(-1/2)}_{a_1}(a_2) = \int dx \{a_1(x,t)\,a_2(x,t)\}^{1/2}. \tag{3.4}$$

Because of (3.2), the degradation functions with $-1 \leq n \leq 0$ are always finite. For other values of n the functions may initially be infinite, corresponding to one of the fields being zero in a part of x-space. The degradation functions $D^{(0)}$ and $D^{(-1)}$ are equal to unity, representing only normalization. At these values of n the entropies appear. Thus, consider the relative entropy

$$S_{a_1}(a_2) = \int dx\, a_1(x,t) \log \frac{a_2(x,t)}{a_1(x,t)}. \tag{3.5}$$

It is alternatively given by

$$S_{a_1}(a_2) = -\frac{1}{n}(D_{a_1}^{(n)}(a_2) - 1)|_{n\to 0}. \tag{3.6}$$

Beside the familiar entropy (3.5) and the symmetric function $D^{(-1/2)}$ in (3.4), special mention should be made of one further degradation function. If the order is $n = 1$ in (3.1), one gets the simple result

$$D_{a_1}^{(1)}(a_2) = \int dx \frac{\{a_1(x,t)\}^2}{a_2(x,t)} = 1 + \int dx \frac{\{a_1(x,t) - a_2(x,t)\}^2}{a_2(x,t)}.$$

This function is used extensively in mathematical statistics,[8,6] and is often called the χ^2-function. The field a_1 is then—in the discrete case—a measured frequency, while a_2 is a probability field.

Some inequalities are immediately found for the degradation functions. They are all equal to unity if and only if $a_1 \equiv a_2$, and generally

$$\left.\begin{array}{l} D_{a_1}^{(n)}(a_2) \geq 1, \quad \text{for} \quad n > 0 \quad \text{or} \quad n < -1, \\ 0 \leq D_{a_1}^{(n)}(a_2) \leq 1, \quad \text{for} \quad -1 < n < 0. \end{array}\right\} \tag{3.7}$$

This may be shown by means of an auxiliary function $f_n(\xi)$, where n is a real number,

$$f_n(\xi) = \xi^{n+1} - (n+1)(\xi - 1) - 1, \quad 0 \leq \xi \leq \infty, \tag{3.8}$$

so that $f_n = 0$ for $\xi = 1$. Obviously, when $\xi \neq 1$,

$$\left.\begin{array}{l} f_n(\xi) > 0, \quad \text{if} \quad n > 0 \quad \text{or if} \quad n < -1, \\ f_n(\xi) < 0, \quad \text{if} \quad -1 < n < 0. \end{array}\right\} \tag{3.9}$$

Since $D_{a_1}^{(n)}(a_2) = \int dx\, a_2 f_n(a_1/a_2) + 1$, and since the D-functions are positive, the inequalities (3.7) follow from (3.9). It is seen from (3.7) and (3.6) that $S_{a_1}(a_2) \leq 0$.

Time dependence

Consider equations of motion of type of (1.2) in a continuum space with arbitrary dimensionality, cf. also SSD,

$$\frac{\partial}{\partial t} a(x,t) = \int dy \{ G(x,y,t) a(y,t) - G(y,x,t) a(x,t) \}, \tag{3.10}$$

where G is non-negative. In case of a differential equation in space, it can at most be of second order, i.e. of type of a diffusion equation. The bonds on the possible linear equations (as expressed by (3.10) with $G \geq 0$) arise when $a(x,t)$ is required to remain non-negative and to have conservation (3.2). Demand, for simplicity, that the system is indivisible, which means that any point x' within the system communicates with any other point x'', so that it cannot be subdivided into independent parts.

We ask for the time derivative of a degradation function (3.1). It contains the time derivatives $\dot{a}_1(x,t)$ and $\dot{a}_2(x,t)$, for which we insert the values given by (3.10). If $G(y,x,t)$ is taken outside as a common factor, the function f_n from (3.8) obtains directly, and we get

$$\frac{\partial}{\partial t} D^{(n)}_{a_1(x,t)}(a_2(x,t)) = -\int dx \int dy\, G(y,x,t) a_1(x,t) \left\{ \frac{a_1(y,t)}{a_2(y,t)} \right\}^n \frac{1}{\xi} f_n(\xi), \tag{3.11}$$

where

$$\xi = \frac{a_1(x,t) a_2(y,t)}{a_2(x,t) a_1(y,t)}. \tag{3.12}$$

It follows then from (3.9) that, unless $a_1 \equiv a_2$,

$$\left.\begin{aligned} &\frac{\partial}{\partial t} D^{(n)}_{a_1}(a_2) < 0, \quad \text{for} \quad n > 0 \quad \text{or} \quad n < -1, \\ &\frac{\partial}{\partial t} D^{(n)}_{a_1}(a_2) > 0, \quad \text{for} \quad -1 < n < 0, \\ \text{and} \quad &\frac{\partial}{\partial t} S_{a_1}(a_2) > 0. \end{aligned}\right\} \tag{3.13}$$

The above demand of an indivisible system is a sufficient condition for the validity of (3.13) but not by far a necessary condition. A weaker, and still sufficient, condition is that for any pair (x', x'') at least one of the points communicates with the other one. This includes one-way systems like (5.7). In any case, equation (3.13) has rather general validity in statistical dynamics, including time-dependent equations of motion and other systems without an equilibrium. It applies for Brownian motion, and the only notable exception is a first order differential equation in the space x. This is essentially the Hamiltonian equations of motion in phase space, for which all degradation functions remain constant in time (cf. SSD).

Ambiguity of absolute measure of information

Consider the question of entropy as a measure of information. For definiteness suppose that we are concerned with a discrete variable, $j = 1, 2, \ldots, n$, with corresponding probabilities p_j, and that to these belong an absolute measure of information equal to H, where $-H$ is statistical entropy, $H = \sum_j p_j \log p_j$, cf. e.g., SHANNON[17] or JAYNES[9]. Now, it is perfectly permissible to let any equation of motion, such as (1.2) or (3.10), act upon the p_j. This means that there is a transmission through some medium with a slight smearing of the distribution in question, and it must be demanded that the measure of information cannot increase by such processes. In order to see clearly the ambiguity in H and in $\partial H/\partial t$, introduce another function $s_p(P) = -\sum_j p_j \log(p_j/P_j)$. Put $P_j = 1/n$, so that $s_p(P)$ is equal to $-H$ plus a fixed number ($\log n$) for any value of p_j. We find the time behaviour of $s_p(P)$ by letting both p_j and P_j change with time according to the same equations of motion (3.10). Then we have a function which can only increase with time, according to (3.13). Returning to the original H, i.e. a function only of p_j, we observe that H does not necessarily decrease; it may just as well increase. This implies that H cannot be used as an unambiguous measure of information. The relativity in entropy is also seen easily for a continuum variable, x, already because arbitrariness in the choice of variable (replace x by e.g., $y = x^3$) necessitates a comparison of $p(x)$ with another field, $P(x)$.

For physical systems a definite description can obtain. Thus, if the equations of motion are time-independent and the system is confined to an energy shell, there may be only one equilibrium distribution, i.e. $P =$ const. within available phase space or quantum states. Entropy can then measure a distribution relative to equilibrium. But just for this reason entropy does not determine the equilibrium distribution (in contrast to the Θ-function, cf. below).

The above does not mean that the results in the theory of communication, as based on an H-function for coding frequencies, are in error but only that they can not be used universally, in particular as regards connection to entropy. The criticism applies, however, if one turns the tables and tries to use information theory as a starting-point for statistical mechanics or measurements.[2, 11] In such attempts JAYNES[9] has introduced a further recipe of an a priori distribution, based on absolute entropy and with connection to Bayesian concepts[14, 10, 5]. ROWLINSON[16] mentions some shortcomings of this a priori distribution, exemplified by the die of JAYNES.

Quite apart from the above lack of uniqueness of entropy as absolute measure of information, there are other deficiencies in this measure. For it is not clear beforehand why entropy should be singled out to the exclusion of the other degradation functions, which all have the same general properties (additivity for independent fields, and composition rules). On the contrary, we found previously that statements of the field from measurements contain not only relative entropy but other relative degradation functions as well.

The Θ-function

The degradation functions are quite general functions of a field, based only on separability for independent fields. They are not necessarily connected with time dependence of a field or with any equation of motion (cf. e.g. the χ^2-function in mathematical statistics). For some purposes it is a disadvantage that they are relative functions, measuring one field with respect to another one. This circumstance is sometimes obscured when a well-defined equilibrium field exists.

It may thus be well-advised to look for functions which are absolute measures of fields, even though their applicability be less general. I shall consider an interesting function of this kind, to be called the Θ-function.

Let there be a field $a(x,t)$, following an equation of motion of type of (3.10), for instance. Suppose that the equation of motion is time-independent, i.e. G in (3.10) does not depend on t. This is clearly a basic situation for systems in physics. Consider a degradation function of n'th order, measuring $a(x,t)$ with respect to the field taken a time τ later, $a(x,t+\tau)$. In the limit of small values of τ one obtains by expansion

$$D^{(n)}_{a(x,t+\tau)}(a(x,t)) = 1 + \frac{n(n+1)}{2}\tau^2\Theta(a(x,t)) + \ldots, \tag{3.14}$$

where Θ is given by

$$\Theta(a(x,t)) = \int dx \frac{\{\dot{a}(x,t)\}^2}{a(x,t)}. \tag{3.15}$$

When (3.10) is introduced in (3.15), Θ is seen to be explicitly a function of one field only, in contrast to the degradation functions. It follows directly from (3.15) that Θ is additive for independent fields; when $a = a_1(x,t)a_2(y,t)$ then $\Theta(a) = \Theta(a_1) + \Theta(a_2)$. This property is inherited from the degradation functions through (3.14).

Clearly, Θ is larger than or equal to zero, the equality sign holding only in equilibrium. Moreover, the degradation functions $D^{(n)}$ were shown to change monotonically with time towards 1. It therefore follows from (3.14) and (3.13) that Θ as a function of time decreases towards zero, if G in (3.10) is independent of t,

$$\frac{\partial}{\partial t}\Theta(a(x,t)) < 0, \quad \text{unless} \quad a(x,t) = a^0(x). \tag{3.16}$$

An obvious application of Θ is therefore, inserting the equation of motion in (3.15), to find the equilibrium field by variational methods, $\delta\Theta = 0$. It is not the aim here, however, to study such problems but only to point out the noteworthy properties of the Θ-function.

§ 4. Dependent Fields

In the previous case of independent fields there was for instance a constant source of the field, and one could make an unlimited number of measurements, thereby improving the knowledge of the field.

The case of a dependent field is in some respects quite different. It affords further insight in physical problems and has connection to measurements as well as to basic theoretical concepts. Measurements of a dependent field may influence strongly the value of the field. Thus, one may make an observation on a Brownian particle, e.g., by ascertaining its position, and thereby obtain new statements as to its behaviour in time and as to the results of other measurements. When a measurement is made, it can be of interest to follow the system both forwards and backwards in time. Measurements of dependent fields may alternatively be considered as preparation of a specific configuration of the system, being thus part of an experimental setup.

It is convenient to make a separation between complete and incomplete measurements of a dependent field. In a complete measurement all coordinates of the system are recorded exactly. Incomplete measurements may observe all coordinates in an approximate manner, or may record exactly a few of the coordinates only.

I employ the following terminology. The field in the absence of measurements is called the original field. The field as modified by measurements is the dependent field, labelled by a star. The dependent field after the measurement is called the subsequent field, whereas the dependent field before the measurement is described as the prior field. If one wishes to visualize these concepts in a simple way, he may suppose that the systems measured have labels so that they can be recognized at all times.

In the following I consider the general case of continuum variables, with discrete variables as an obvious specialization. Suppose that the normalized field, at time $t = 0$, is $a(x,0)$. It obeys the equations of motion (1.1), (1.2), or (3.10), so that for $t \geq 0$

$$a(x,t) = \int dx'\, T(x,t;x',0)\, a(x',0). \tag{4.1}$$

Complete measurement

Suppose that a measurement is made at time t_1 with the unique result that the particle is at position x_1 (for instance a certain point in phase space). This complete measurement implies of course an unwarranted accuracy, but that is of no consequence in the present derivation. In fact, one might instead consider a probability statement with a certain width around x_1. Note also that in the corresponding discrete case it is completely justified to suppose that the system is observed at a definite position k.

The distribution of the system as determined by the measurement we call $a^*(x, t)$ so that

$$a^*(x,t_1) = \delta(x - x_1). \tag{4.2}$$

The probability of obtaining the measurement (4.2) is represented by the value of the original field, $a(x_1, t_1)$ from (4.1).

It is easy to find the field subsequent to the measurement, since by the equations of motion (4.1) acting on (4.2) one gets

$$\left.\begin{aligned} a^*(x_2,t_2) &= \int dx'\, T(x_2,t_2;\, x',t_1)\, a^*(x',t_1) \\ &= T(x_2,t_2;\, x_1,t_1), \qquad t_2 \geq t_1. \end{aligned}\right\} \tag{4.3}$$

Eq. (4.3) is the probability of obtaining x_2 at time t_2 if one has x_1 at t_1. If we multiply (4.3) by the probability $a(x_1, t_1)$ of x_1 at t_1, we obtain the combined probability of the two events

$$P(x_2,t_2,x_1,t_1) = T(x_2,t_2;\, x_1,t_1)\, a(x_1,t_1), \quad t_2 \geq t_1. \tag{4.4}$$

The result (4.4) may be extended to any number of subsequent measurements by multiplication with the appropriate propagators $T(x_{i+1}, t_{i+1};$

x_i, t_i). Therefore, one is concerned with a Markov chain[7], as is characteristic of complete measurements of a dependent field. But the more common case of incomplete measurements of a dependent field (cf. below) does not have this Markov property in full.

We next ask for the field backwards in time, as modified by the measurement at t_1, and call it the prior field. It is already determined by the previous considerations. The total probability of the two events at times t_1 and t_2 is given by (4.4) and we can obtain $t_2 < t_1$ by exchanging indices 1 and 2 in this formula, i.e. $T(x_1, t_1; x_2, t_2)a(x_2, t_2)$. The undisturbed probability of x_1 at t_1 with the original field is $a(x_1, t_1)$. By dividing into the product we obtain the probability of x_2 at t_2 if x_1 at t_1, i.e. the prior field

$$a^*(x_2, t_2) = \frac{1}{a(x_1, t_1)} T(x_1, t_1; x_2, t_2)\, a(x_2, t_2), \quad t_2 \leq t_1. \tag{4.5}$$

Note that $a^*(x_2, t_2)$ is normalized to unity. The formula (4.5) is also familiar for Markov chains (cf. DOOB[7]). Observe also that, unless a is the equilibrium field, it may cease to exist when $t_2 \to -\infty$, so that t_2 in (4.5) attains a lower limit too.

Time reversibility in equilibrium

Let us suppose, first, that the equations of motion are time-independent, so that $T(x_2, t_2; x_1, t_1) = T(x_2, x_1, t_2 - t_1)$. Second, let the original field be the equilibrium field, $a(x, t) = a^0(x)$, and thus independent of time. In fact, this is usually the most convenient way of preparing a system in a well-defined state; if it is left undisturbed for some time the equilibrium is attained with any desired degree of accuracy. When the original field is $a^0(x)$ the prior field (4.5) becomes

$$a^*(x_2, t_2) = \frac{1}{a^0(x_1)} T(x_1, x_2, t_1 - t_2)\, a^0(x_2), \quad t_2 \leq t_1. \tag{4.6}$$

When $t_2 \to -\infty$, the prior field (4.6) approaches the equilibrium field $a^0(x_2)$, because $T(x_1, x_2, \infty) = a^0(x_1)$. Likewise, the subsequent field (4.3) tends to $a^0(x_2)$ for $t_2 \to +\infty$.

The case considered here has particular interest because it allows a new approach to a familiar problem in the discussion of statistical mechanics near equilibrium. In that connection one often makes use of the conceptions of microscopic reversibility and macroscopic irreversibility. The Onsager relations[3,15] between thermodynamic parameters are then considered as a consequence of microscopic reversibility, the latter being due to time reversibility of the Hamiltonian equations of motion.

The present equations of motion of statistical dynamics are much simpler in having no need of distinction between a macroscopic and a microscopic region, the motion being always irreversible. We can, however, now consider the question of effective time reversibility in equilibrium for a dependent field, on the basis of (4.6) and (4.3). To this end, consider the dependent field at times $t_2 = t_1 \pm \tau$,

$$\left.\begin{aligned} a^*(x_2, t_1 + \tau) &= T(x_2, x_1, \tau), \\ a^*(x_2, t_1 - \tau) &= \frac{1}{a^0(x_1)} T(x_1, x_2, \tau)\, a^0(x_2). \end{aligned}\right\} \quad (4.7)$$

We demand effective time reversibility in equilibrium, i.e. always

$$a^*(x_2, t_1 + \tau) = a^*(x_2, t_1 - \tau), \quad (4.8)$$

and obtain from (4.7) the condition

$$T(x_2, x_1, \tau) \cdot a^0(x_1) = T(x_1, x_2, \tau)\, a^0(x_2) \quad \text{for all} \quad \tau > 0. \quad (4.9)$$

The condition (4.9) requires that — in equilibrium — the rate of transition from any space point to any other point during any finite time τ is equal to the opposite rate. This property was called spatial reversibility in SSD. It was shown there that (4.9) is completely equivalent to a demand of spatial reversibility of the elementary transition rates, cf. (3.10),

$$G(x_2, x_1)\, a^0(x_1) = G(x_1, x_2)\, a^0(x_2) \quad (4.10)$$

for all x_1, x_2. It does not matter if $G(x_1, x_2) = 0$ for many $x_2 \neq x_1$, or for all $x_2 \neq x_1$, i.e. the limit where differential equations obtain from (3.10). The demand is merely that the system is indivisible, and thus has a unique equilibrium $a^0(x)$, and that (4.10) is fulfilled.

The demand of effective time reversibility in equilibrium leads to, e.g., the Onsager relations. But it is not necessarily connected with time reversibility of the equations of motion. On the contrary, according to (4.10) it poses a simple condition on the equations of motion. This condition is easily fulfilled by differential equations of motion, like Brownian motion. The situation is illustrated by the two following examples.

Example; Brownian motion

Consider Brownian motion of a particle in momentum space without external forces.[4] In this case momentum space gives a complete account of the behaviour, if we abstain from asking about the motion in coordinate space. Assume therefore that the equation of motion is

$$\frac{\partial}{\partial t} a(p,t) = \frac{\partial}{\partial p} D \left\{ \frac{\beta p}{M} + \frac{\partial}{\partial p} \right\} a(p,t), \tag{4.11}$$

where D and β are constants. The equilibrium of (4.11) is given by the Maxwell distribution

$$a^0(p) = (\beta/2\pi M)^{1/2} \exp(-\beta p^2/2M). \tag{4.12}$$

According to SSD, p. 29, the equation (4.11) leads to spatial reversibility. In order to see this explicitly, find the propagator $T(p,p_0,\tau)$ belonging to (4.11). It is

$$T(p,p_0,\tau) = \left\{ \frac{\beta}{2\pi M(1-e^{-2\lambda\tau})} \right\}^{1/2} \exp\left\{ -\frac{\beta}{2M} \frac{(p-p_0 e^{-\lambda\tau})^2}{1-e^{-2\lambda\tau}} \right\}, \tag{4.13}$$

where the damping time is $\lambda^{-1} = M/(D\beta)$.

It follows from (4.13) and (4.12) that

$$\frac{1}{a^0(p)} T(p,p_0,\tau) = \frac{1}{a^0(p_0)} T(p_0,p,\tau), \tag{4.14}$$

i.e. spatial reversibility in momentum space.

Now, if the particle is measured to have momentum p_0 at a certain time t, then (4.13) represents its distribution in p at a time $t + \tau$. But if the original distribution was the equilibrium (4.12), then it follows from (4.14), (4.6) and (4.3) that the distribution of the measured particle is also (4.13) at a time $t - \tau$. There is thus time reversibility in equilibrium because of the reversibility in momentum space for the time irreversible equation of motion (4.11). With this example we are getting close to statistical dynamics in phase space, where the Hamiltonian equations of motion play a part. In fact, with a view to this we can formulate another symmetry property of (4.11). Note that in (4.13)

$$T(-p,-p_0,\tau) = T(p,p_0,\tau). \tag{4.15}$$

Therefore (4.14) becomes, because of (4.12),

$$\frac{1}{a^0(p)} T(p,p_0,\tau) = \frac{1}{a^0(-p_0)} T(-p_0,-p,\tau). \tag{4.16}$$

This result is the one which remains valid in statistics in phase space.

Counterexample: Multiple scattering with damping

It is instructive to consider a case without spatial reversibility, for continuum variables. The purpose is not merely to show that mathematically simple counter-examples may be found. It is, rather, to make clear that absence of reversibility in, e.g., momentum space is not only possible but even quite common in familiar problems from physics.

Small angle multiple scattering is equivalent to motion in transverse momentum space. The previous paper, SSD, contains several exact solutions of such integral equations. The simplest case of this kind corresponds, approximately, to classical scattering by R^{-2}-potentials. Let us in this case introduce a damping of the transverse motion, proportional to transverse momentum and due to slowing-down effects. This is not unlike what may happen in e.g., proper channelling[13].

The desired equation of motion in momentum space is, if we simplify to the one-dimensional case,

$$\frac{\partial}{\partial t}a(p,t) = \lambda\frac{\partial}{\partial p}\{pa(p,t)\}+C\int_{-8}^{\infty}\frac{d\eta}{\eta^2}\{a(p+\eta,t)-a(p,t)\}, \tag{4.17}$$

where p is the small transverse momentum, and η the change of transverse momentum by scattering. The equilibrium belonging to (4.17) is

$$a^0(p) = \frac{C/\lambda}{p^2+\pi^2(C/\lambda)^2}. \tag{4.18}$$

It is not difficult to find the propagator $T(p,p_0,\tau)$ belonging to (4.17),

$$T(p,p_0,\tau) = \frac{(1-e^{-\lambda\tau})\cdot(C/\lambda)}{(p-p_0e^{-\lambda\tau})^2+\pi^2(1-e^{-\lambda\tau})^2(C/\lambda)^2}, \tag{4.19}$$

which formula has several features in common with the corresponding one for Brownian motion, (4.13). But there is not spatial reversibility, since (4.18) and (4.19) do not fulfill (4.14). In fact, suppose that the system is in equilibrium, and that at t the momentum is measured to be p_0. The subsequent field, (4.3), is then given by (4.19)

$$a^*(p,t+\tau) = T(p,p_0,\tau), \tag{4.20}$$

but the prior field is, according to (4.6),

$$a^*(p,t-\tau) = \frac{p_0^2+\pi^2(C/\lambda)^2}{p^2+\pi^2(C/\lambda)^2}\cdot\frac{(1-e^{-\lambda\tau})\cdot(C/\lambda)}{(p_0-pe^{-\lambda\tau})^2+\pi^2(1-e^{-\lambda\tau})^2(C/\lambda)^2}. \tag{4.21}$$

The formulae (4.21) and 4.20) are quite dissimilar; note in particular that, for $p\to\infty$, $a^*(p,t-\tau)/a^*(p,t+\tau)\to 0$. This result illustrates also how transient equilibrium distributions in physical systems may fail to give effective time reversibility, when integro-differential equations of motion are involved.

Incomplete measurement

As a supplement to the previous complete measurement of a dependent field let us discuss briefly the consequences of incomplete measurements. As an example, a number of particles may perform Brownian motion, the instantaneous state of each particle being given by a point in phase space. An incomplete measurement might be to record only one momentum component of a particle. This case being quite simple, I shall instead look into the alternative problem where a measurement is only approximate.

Let the original field be given by (4.1) as before. Consider an incomplete measurement in the sense that it gives only a probability statement about the coordinates of the system. For definiteness, suppose that one has a counter measuring at time t_1, with its centre placed at x_1. If a particle passes the point x at t_1, the counter gives off a signal with probability $f(x - x_1)$. Only the relative probabilities of signals matter for the present, so assume that $\int dx f(x - x_1) = 1$. But it should be realized that successive measurements imply a decrease which can have serious consequences.

We ask for the value of the prior field $a^*(x_2, t_2)$, $t_2 < t_1$, when an observation is made with the counter at time t_1, given the original field $a(x,t)$. If a particle starts from x_2 at t_2 its probability of reaching x is $T(x, t_1, x_2, t_2)$. Its probability of being recorded is therefore $\int dx f(x - x_1) T(x,t_1; x_2, t_2)$. Moreover, the original probability of arriving at x_2, t_2 is $a(x_2, t_2)$ and, if this is multiplied into the integral, one gets the total probability of recording a particle having passed through x_2, t_2. Now, this is also—apart from a constant of normalization—the probability that the particle was at x_2, t_2, when it is recorded at time t_1; in fact, the latter result expresses merely the theorem of Bayes[7,10,14]. The prior field is therefore

$$a^*(x_2, t_2) = C^{-1} \int dx f(x - x_1) T(x, t_1; x_2, t_2) a(x_2, t_2), \quad t_2 \leq t_1, \tag{4.22}$$

with

$$C = \int dx_2 \int dx f(x - x_1) T(x, t_1; x_2, t_2) a(x_2, t_2) = \int dx f(x - x_1) a(x, t_1). \tag{4.23}$$

When the two times are equal, $t_2 = t_1$, (4.22) becomes, since $T(x,t_1; x_2,t_1) = \delta(x - x_2)$,

$$a^*(x_2, t_1) = C^{-1} f(x_2 - x_1) a(x_2, t_1), \tag{4.24}$$

and this result is more easily obtained by a direct argument.

By means of the propagator (4.1) acting on (4.24) the subsequent field obtains,

$$a^*(x_2, t_2) = C^{-1} \int dx\, T(x_2, t_2; x, t_1) f(x - x_1) a(x, t_1), \quad t_2 \geq t_1. \tag{4.25}$$

In a general sense, therefore, the results for incomplete measurements of dependent fields do not deviate from those for complete measurements, except in being more complicated. In particular, the results concerning effective time reversibility in equilibrium, as expressed in (4.9) and (4.10), remain valid for incomplete measurements, i.e. when (4.22) and (4.25) hold.

§ 5. Inversion of Probabilities

The direct probability for a discrete variable was illustrated in (2.1) and (2.3), where the probabilities of various events $\bar{N}$ were found when the independent field $\bar{a}$ was given. The problem of inversion consists in finding what statement may be made about the field $\bar{a}$ when some event $\bar{N}$ is observed. This statement is, at most, a probability distribution of the field.

In the following I therefore suppose that no more than the direct probability is known for a complete set of events and for any field. I ask whether an inverse probability follows uniquely from it. We shall find that in some cases there is in fact a unique solution, while in other cases the solution has an uncertainty. This is quite similar to the results in usual inversion problems in mathematics.

It appears necessary to state the basic problems and their solution in some detail, because one may easily be led astray in these questions. In fact, the difficulties met with have led to various schools of thought in mathematical statistics, since the time when Bayes[1] drew attention to the problem. In consequence, a number of concepts of different content are used in the literature. They range from the cautious use of 'likelihood', not conceived as a probability,[8] to the introduction of 'a priori probabilities',[10,14] which are not part of the problem as stated above.

More specifically, the following discussion takes up two major problems. The first one is the question of inversion of probability between continuum variables, to be studied in some detail for one-way variables. The second problem concerns a discrete variable, e.g., a true discrete variable like the number of alpha-particles emitted by a radioactive specimen, or an artificial one created by dividing a continuum variable into a number of intervals for the purpose of measurement. With a discrete variable one does not have a unique inversion of probability but a latitude appears as we shall see.

A third major problem concerns actual interpretation, in a given experiment, of an inversion statement about the field. This problem can be the most intriguing one. Thus, if one asks for a statement concerning an unknown parameter λ, the latter need not be, say, a stochastic quantity since it can have a fixed unknown value. Of course, it can then be difficult to have a realizable frequency interpretation of the probability of λ; but that may occur for direct probabilities too. The more subtle difficulties are connected with other properties of probability, like independence and composition rules.

To sum up: I shall consider merely the well-defined question of what inversion statement is permitted when just the direct probabilities are known. I do not attempt to introduce a systematic and comprehensive theory, selecting instead suitable examples, which also illustrate actual applications. Whereas the aim is discrete variables, I solve first the simple case of one-way continuum variables.

One-way distribution in continuum case, and its inversion

Inversion of probability is a generalization of inversion of a function.* Thus, consider two variables, t and x, and a curve $x = f(t)$ in the t–x plane. The basic case for inversion of the function $f(t)$ obtains when it increases monotonically with t, because then the inversion $t = f^{-1}(x)$ is unique. We may suppose that $0 \leq t < \infty$, that $f(0) = 0$, and that there is no upper bound of $f(t)$; this does not imply a limitation of the results. If $f(t)$ were not monotonically increasing, one would have a more complicated problem of inversion. In particular, if $f(t)$ were constant in an interval $t_1 \leq t \leq t_2$, there would be no unique inversion when $x = f(t_1)$. As we shall see, the one-way variables in probability theory—or in statistical dynamics—are the analogue of monotonically increasing functions.

Consider the general case of a distribution of mass, with density $\varrho = \varrho(x, t)$, where ϱ is defined for $0 \leq t < \infty$, $0 \leq x < \infty$, and $\varrho \geq 0$. If I regard the mass distribution as a probability distribution of x for a given t, I write $P_t(x) \equiv \varrho(x, t)$. The distribution is assumed to have conservation, or

$$\int_0^\infty dx\, \varrho(x,t) = 1, \quad 0 \leq t < \infty. \tag{5.1}$$

It follows from the conservation (5.1) that, at the point x at time t, one may introduce a current $j(x, t)$ as

$$j(x,t) = -\frac{\partial}{\partial t}\int_0^x \varrho(x',t)\,dx' \equiv -\frac{\partial}{\partial t}M(x,t), \tag{5.2}$$

or

* Because of this simple connection I use the term 'inversion' of probability. I should mention that, in mathematical statistics, the word 'inversion' is sometimes used in a different sense.[8, 10]

$$\frac{\partial}{\partial t}\varrho(x,t) + \frac{\partial}{\partial x}j(x,t) = 0. \tag{5.3}$$

I shall suppose that, for all t and x, the function $j(x, t)$ in (5.2) is non-negative,

$$j(x,t) > 0, \quad \text{when} \quad \varrho(x,t) > 0. \tag{5.4}$$

This means that the distribution $\varrho(x, t)$ always moves in the direction of the positive x-axis, where motion stands for change when t increases. Eq. (5.4) therefore implies that x is a one-way variable, and that the distribution behaves similarly as the monotonous function $f(t)$.

Make now the following three assumptions as to the density $\varrho(x, t) \equiv P_t(x)$. First, suppose that $\varrho(x, 0) = \delta(x)$, so that at time $t = 0$ the distribution starts at the origin. Second, assume that there is not a finite probability placed on the t-axis outside the origin, i.e. $\varrho(x, t)$ can not contain a component of type of, say, $\delta(x)\cdot e^{-t/\tau}$. Third, assume for convenience that $\varrho(x, t \to \infty) \to 0$ at any fixed x, so that the distribution moves to infinitely large values of x when $t \to \infty$. The third demand, together with (5.2), implies that

$$\int_0^\infty dt\, j(x, t) = 1. \tag{5.5}$$

It is thus plausible that $j(x, t)$ is a probability density. Actually, when (5.4), (5.5) and the three assumptions are fulfilled, there exists a probability density of t for given x

$$P_x(t) \equiv j(x,t) = -\frac{\partial}{\partial t}\int_0^x dx'\,\varrho(x',t) = -\frac{\partial}{\partial t}M(x,t). \tag{5.6}$$

I call $P_t(x)$ and $P_x(t)$ the direct and inverse densities connecting one-way variables x and t. The above curve $x = f(t)$ is a rather special example of this kind, since $P_t(x) = \delta(x - f(t))$ and $P_x(t) = f'(t)\delta(x - f(t)) \geq 0$.

Let me show, by a simple argument, that (5.6) is the inverse probability. Thus, approximate the density $\varrho(x, t)$ by a set of N successive curves $f_i(t)$, all starting at the origin, increasing monotonically with t without intersection, and tending to infinity for $t \to \infty$. Each of the curves is given a probability weight $1/N$, so that the total weight is 1. We may determine $f_i(t)$ by $i/N = \int_0^{f_i} \varrho(x,t)dx \equiv M(f_i,t)$, whereby the previous assumptions secure that the curves have the desired properties. The total density belonging to the set of curves is $P_t^N(x) = \sum_{i=1}^{N} \delta(x - f_i(t))/N$, but this can be inverted to $P_x^N(t) =$

$\sum_i f_i'(t)\delta(x-f_i(t))/N$, where $f_i'(t)>0$ since $j(x,t)$ is positive. In the limit of $N\to\infty$, the inverse probability $P_x^N(t)$ becomes $P_x(t)$ in (5.6) which then is the inverse of $P_t(x)$. In order to have uniqueness we must in particular require that the derivative of the first curve, $f_1'(t)$, remains different from zero for any value of N; but that is a consequence of the second assumption above. If this assumption were not fulfilled, one would meet with problems like those belonging to discrete variables (cf. p. 35). Note, finally, that when $P_x(t)$ in (5.6) is the inverse of $P_t(x)$, then $P_t(x)$ is also the inverse of $P_x(t)$.

One-way equation of motion

Consider now an example of equations of motion for one-way variables. Suppose that the distribution $\varrho(x,t)$, with initial condition $\varrho(x,0)=\delta(x)$, obeys the integro-differential equation

$$\frac{\partial}{\partial t}\varrho(x,t) = \int_0^\infty g(\eta)\,d\eta\{\varrho(x-\eta,t)-\varrho(x,t)\}, \tag{5.7}$$

where $g(\eta)$ is non-negative. Accordingly, $\varrho(x,t)$ remains non-negative, and it also has conservation, $\int dx\varrho(x,t)=$ const. The equation (5.7) is somewhat specialized in being invariant towards displacements along both t-axis and x-axis (cf. SSD, in particular § 6). Since only positive values of η occur in (5.7), it is obvious that the distribution always moves in the positive x-direction and (5.4) is fulfilled.

There are some conditions on $g(\eta)$ in (5.7). In order to have convergent results, so that ϱ does not move promptly to infinity, there are a few demands on $g(\eta)$. It is required that $q_\varepsilon=\int_\varepsilon^\infty g(\eta)\,d\eta$ has a finite value but, when $\varepsilon\to 0$, q_ε is allowed to diverge. This corresponds to a collision cross section which diverges for soft collisions, if we consider $g(\eta)d\eta$ as being proportional to a differential collision cross section. The divergence can not be too strong, because $\int_0^\varepsilon \eta g(\eta)\,d\eta$ must have a finite value so as to avoid prompt motion to $x=\infty$. The basic solutions of (5.7) are the propagators, i.e. functions which initially are $\varrho(x,t=0)=\delta(x)$, corresponding to the first assumption. They have the property $\varrho(x,t_1+t_2)=\int_0^x\varrho(x-x',t_1)\,\varrho(x',t_2)dx'$. In order that the second assumption on p. 30 be fulfilled, so that no part of the distribution remains on the t-axis, there is a requirement of $g(\eta)$. We must demand

$$q_\varepsilon = \int_\varepsilon^\infty g(\eta)d\eta \to \infty \quad \text{for } \varepsilon \to 0, \tag{5.8}$$

so that the corresponding transition cross section diverges. This is obvious, since if q_0 were finite, part of the distribution would remain on the t-axis, in fact $\exp(-q_0 t)\delta(x)$.

Explicit solution of inversion

We have thus found that the distribution (5.7) with the condition (5.8) can be inverted by eq. (5.6). Consider a specialized case of (5.7), where $g(\eta)$ obeys a power law,

$$g(\eta) = C_n/\eta^{1+n}, 0 < n < 1. \tag{5.9}$$

It is clear, for dimensional reasons, that (5.9) leads to distributions of the kind $P_t(x) = \varrho(x, t) = x^{-1}\varphi_n(x^n/C_n t)$, which is a so-called stable distribution. In this case the inverse probability is immediately obtained from (5.6),

$$P_x(t) = \frac{x}{nt}P_t(x). \tag{5.10}$$

In this simple case $P_x(t)$ is not far from being proportional to $P_t(x)$. This is due to the simple assumptions in (5.7) and (5.9). But it is worth noting that the two probability distributions are not each others 'likelihood'.

Consider a particular choice of n in (5.9). As we shall see, the case of $n = 1/2$ has particular interest. According to SSD one gets the propagator, with $C_{1/2} = C$,

$$P_t(x) = \frac{Ct}{x^{3/2}}\exp\left(-\frac{\pi C^2 t^2}{x}\right). \tag{5.11}$$

The inverse probability is found from (5.10),

$$P_x(t) = \frac{2C}{x^{1/2}}\exp\left(-\frac{\pi C^2 t^2}{x}\right). \tag{5.12}$$

Eq. (5.11) may represent the probability distribution of total energy loss x for an energetic ion which passes through a foil of thickness t, suffering elastic collisions with atoms in the foil. The differential probability of an individual energy loss between η and $\eta + d\eta$ is $Cdtd\eta/\eta^{3/2}$, cf. (5.9), for passage through a distance dt. The distribution (5.11) of total energy loss x for given thickness t is a peak of moderate width. If one measures a given total energy loss and the thickness is unknown, he finds a wide probability distribution of thickness. It should be emphasized here that interpretation of inversion experiments based on (5.11), (5.12), (5.13), and (5.13′) contains many subtleties, unnecessary for the derivation in the following sections however.

The distribution (5.12) is quite familiar if the problem is turned around. Suppose one has a one-dimensional diffusion process with diffusion constant $D = 1/(4\pi C^2)$, t being the numerical value of the distance from the starting-point, while x is the time variable. Then the Gaussian (5.12) is the direct probability distribution of the distance t for a known value of the time x, or of Dx. The inverse probability is now (5.11), giving the distribution of the time x, or of $Dx = \sigma^2/2$, if one measurement gives the distance t from the origin.

Returning to the definite example of one particle at depth t in a substance having suffered an energy loss x, it is quite obvious that knowledge of t gives a distribution (5.11) of energy loss x, and knowledge of x gives a distribution (5.12) of range t. But suppose in the former case that x has a fixed unknown value, and that ν measurements are made, giving $t_1, t_2, \ldots, t_\nu$. This may be imagined to happen, somewhat oversimplified, if the track of each particle remains visible until an energy x is lost, the threshold x being unknown. Now, the set of ν measurements may be considered as a single measurement, and in the present case the formulae are simple if described in a ν-dimensional Euclidean space. Introduce a length T by $T^2 = \sum_{i=1}^{\nu} t_i^2$. The direct probability of $\bar{t}$ is a function of ν factors and may be expressed by T, i.e. on differential form $2(\pi^{1/2}C/x^{1/2})^\nu \exp(-\pi C^2T^2/x)T^{\nu-1}dT/\Gamma(\nu/2)$. The usual inversion (5.6) leads to

$$P_T(x) = \frac{(\pi C^2T^2)^{\nu/2}}{\Gamma\left(\frac{\nu}{2}\right)} \frac{1}{x^{\nu/2+1}} \exp\left(-\frac{\pi C^2T^2}{x}\right), \qquad (5.13)$$

which formula is the familiar χ^2-distribution. Second, if the thickness of the substance has a fixed unknown value t, and energy losses $x_1, x_2, \ldots x_\nu$ are measured, a differential product probability obtains, as a function of t and ξ, where $\xi^{-1} = \sum_{i=1}^{\nu} x_i^{-1}$. By inversion one gets from (5.6)

$$P_\xi(t) = \left(\frac{\pi C^2}{\xi}\right)^{\nu/2} \frac{2t^{\nu-1}}{\Gamma\left(\frac{\nu}{2}\right)} \exp\left(-\frac{\pi C^2t^2}{\xi}\right), \qquad (5.13')$$

quite similarly to (5.13).

These results, belonging to a well-known distribution, are meant to illustrate the straightforward content of direct and inverse probabilities, as well as the combination of several measurements. Though, in principle, similar calculations may be made for other stable distributions (5.9), they are more difficult in practice.

Consider next another example with wide applicability but of particular interest in connection with discrete variables. Suppose that in (5.7)

$$g(\eta) = \frac{C}{\eta} e^{-\eta}, \tag{5.14}$$

corresponding to (5.9) in the disallowed case $n = 0$, but with an exponential cut-off. The total cross section in (5.14) is infinite, i.e. (5.8) is fulfilled. The formula (5.14) is closely analogous to the differential probability per unit time of emitting electromagnetic quanta of energy $\hbar\omega \to \eta$ by an accelerated charged particle. The desired divergence of the total cross section of (5.14) then corresponds to the so-called infrared 'catastrophe'. Replace in (5.7) the variable x by τ and Ct by μ. The particular solution of (5.14), (5.7) which starts at the origin, i.e. the propagator, is then the gamma density

$$P_{\mu}(\tau) \equiv \varrho(\tau, \mu) = \frac{1}{\Gamma(\mu)} e^{-\tau} \tau^{\mu-1}, \tag{5.15}$$

with an inverse according to (5.6)

$$P_{\tau}(\mu) = \frac{1}{\Gamma(\mu)} \int_{\tau}^{\infty} d\tau' e^{-\tau'} \tau'^{\mu-1} \{\log \tau' - \psi(\mu)\}. \tag{5.16}$$

Discrete variable

As mentioned previously, the case of a discrete variable usually does not allow of a well-defined inversion of probability. There will be a latitude, but the inversion can often be bracketed rather narrowly between two probability distributions.

As a preliminary, consider the Poisson process. For definiteness, suppose that one has a radioactive specimen for which λ is the probability of emission of an α-particle per unit time. Therefore, λ is a measure of the number of radioactive atoms in the specimen, being proportional to this number. Introduce $\tau = \lambda t$ as a dimensionless time variable.

There are two situations with well-defined probability distributions. First, suppose that one records the time instances at which each α-particle is emitted. The starting-point of time is chosen to coincide with the emission labelled zero. A familiar analysis of the probability distribution of emission times, for instance by means of an equation analogous to (5.7), gives

$$\left.\begin{aligned} P_0^e(\tau) &= \delta(\tau), \\ P_m^e(\tau) &= \frac{1}{(m-1)!}\tau^{m-1}e^{-\tau}, \quad m = 1, 2, \ldots\ldots, \end{aligned}\right\} \qquad (5.17)$$

i.e. the gamma distribution. The index e in P indicates that one is concerned with the instant of emission. The distribution (5.17) has the same composition rules as (5.15) but is confined to integers.

If one measures the time t of the n'th emission, eq. (5.17) can give the probability distribution of $\lambda = \tau/t$. Consider an example of this kind. Suppose that one has two specimens of α-emitters, 1 and 2, and wants to determine the unknown fractional mass $\lambda_1/(\lambda_1 + \lambda_2) = a_1$. Two time measurements are made corresponding to emission numbers n_1 and n_2, giving times t_1 and t_2. The separate and independent probability distributions of λ_1 and λ_2 are then found from (5.17), whereby the desired probability distribution of a_1 is obtained. Note that the two times t_1 and t_2 cannot be expected to be equal in magnitude. If they are, the quantity a_1 acquires the beta distribution, as it should be.

Second, the Poisson distribution results if the counter is open during a given time interval t, with a known value of λ, so that the dimensionless time variable, $\tau = \lambda t$, is known. One then asks about the probability of n particles having been emitted during this time. The derivation is well-known and leads to

$$P_\tau(m) = \frac{1}{m!}\tau^m e^{-\tau}, \quad m = 0, 1, 2, \ldots\ldots. \qquad (5.18)$$

This type of measurement is the most common one, for instance with a number of specimens counted during the same time interval. It thus comprises both (2.2) and (2.1), i.e. the cases envisaged in § 2. For definiteness, let now the zero-point of the time interval $\tau = \lambda t$ in (5.18) coincide with the emission of a particle, i.e. the particle with label 0.

The noteworthy property of (5.18) is that there is not unique inversion. The reason is simply that one variable is discrete, and the lack of uniqueness has, in a sense, no connection with the fact that we are concerned with probabilities. Thus, the number m in formula (5.18) means that one is somewhere in the interval $(m, m+1)$. In fact, we have to do with one-way distributions, and thus with distributions in the interval $m \leq \mu < m + 1$ in (5.15). We can therefore introduce inversion of (5.18). The corresponding quantity will be called $\tilde{P}_m(\tau)$, where $\sim$ indicates that the function is not uniquely defined but contains a latitude. In all estimates we get an interval of distributions

$$P^e_m(\tau) \leq \tilde{P}_m(\tau) < P^e_{m+1}(\tau), \qquad (5.19)$$

where the inequalities are symbolic, meaning only that there is a latitude in the index. Thus, it holds in a straightforward sense that averages over $\tilde{P}_m(\tau)$ of increasing functions like τ^s obey inequalities,

$$\int_0^\infty P^e_m(\tau)\tau^s d\tau \leq \int_0^\infty \tilde{P}_m(\tau)\tau^s d\tau < \int_0^\infty P^e_{m+1}(\tau)\tau^s d\tau, \qquad (5.19')$$

because of the one-way property of the variables. It may also easily be shown that $\tilde{P}_m(\tau)$ has a simple composition rule.

Determination of $\bar{a}$ from N-measurement

Clearly, the above method allows a determination of τ_1 and τ_2 if m_1 and m_2 are observed. This gives in fact the inversion statement belonging to formula (2.1). I shall derive this inversion in a more direct way.

Consider a unit interval, $0 \leq \alpha \leq 1$, divided into n parts of length $a_1, a_2, \ldots, a_n, \sum a_i = 1$. The magnitude of the a's is unknown. In an N-measurement there will be N points on the unit interval, each one with equal probability everywhere, and each one independently of the others. The probability of recording $N_1, N_2, \ldots, N_n$ points in the intervals is evidently given by (2.1). Now, disregard for a while the division in intervals and consider only the distribution of the N points in the unit interval. Let the points be labelled from 1 to N corresponding to increasing values of α. If we ask for the distance between point s and point $s+m$, we find that it has a probability distribution in length $P_m(\alpha)\,d\alpha$, where α represents $\alpha_{s+m} - \alpha_s$, and

$$P_m(\alpha)\,d\alpha = \frac{N!}{(N-m)!\,(m-1)!}(1-\alpha)^{N-m}\alpha^m\frac{d\alpha}{\alpha}, \qquad (5.20)$$

the so-called beta distribution. Consider next the unknown length a_i on which N_i points are placed. The interval a_i must be greater than the distance between the first and last points within it, i.e. $m = N_i - 1$ in (5.20) but smaller than the distance between the points just outside it, or $m = N_i + 1$ in (5.20). The uncertainty may be narrowed by switching the intervals. Thus, interchange a_i and $1 - a_i$, as well as N_i and $N - N_i$, so that (5.20) applies with m in the interval $(N_i, N_i + 2)$. Together, the two results imply that the original interpretation of formula (5.20) requires

$$N_i < m < N_i + 1. \tag{5.21}$$

One can in analogy to (5.20) perform a complete discussion with the $n - 1$ variables. But in fact this is not necessary, because the distribution of, say, $a_1 + a_2$ must be the same, whether we consider it as one interval with count $N_1 + N_2$ or as two intervals a_1 and a_2, afterwards integrating over one of the variables for a fixed sum. In all, we therefore obtain from (5.20) and (5.21), not a uniquely defined probability, but a distribution $\tilde{P}_{\bar{N}}(\bar{a})$ bounded by probability distributions, which may be formulated as follows

$$\left.\begin{aligned} &\tilde{P}_{\bar{N}}(\bar{a}) \frac{da_1}{a_1} \cdot \cdot \cdot \cdot \cdot \frac{da_n}{a_n} \delta(\sum_i a_i - 1) = \\ &= a_1^{N_1} \cdot \cdot \cdot \cdot \cdot a_n^{N_n} \cdot \frac{da_1}{a_1} \cdot \cdot \cdot \cdot \cdot \frac{da_n}{a_n} \cdot C a_1^{\xi_1} \cdot \cdot \cdot \cdot \cdot a_n^{\xi_n} \delta(\sum_i a_i - 1), \end{aligned}\right\} \tag{5.22}$$

where $\sum_i \xi_i = 1$ and $0 < \xi_i < 1$. This formula* is applied in § 2, p. 10ff. The above-mentioned additivity of the a_i is seen to be fulfilled by (5.22). This is the same additivity as is contained in the direct probability (2.1). The present description therefore does not have awkward consequences of the kind resulting from LAPLACE's rule of succession.[10)]

The above discussion of inversion is limited to one group of problems. By and large it seems not to be in disagreement with the ideas of R. A. FISHER[8)], as expressed in particular by the concepts of likelihood and fiducial probability. The proper inversion problems cover both of these concepts at the same time. On the basis of well-defined one-way distributions I have attempted to obtain quantitative statements of inversion, whereas a likelihood concept can lead to only qualitative statements, in the neighbourhood of the present ones though.

The theorem of Bayes applies when one is concerned definitely with conditional probabilities, as for dependent fields in § 4. To extend this theorem to all cases of inversion, by claiming a priori probabilities, would

* Note that the formula belongs to a total interval for which the end-points are uniquely defined; in other cases the sum $\sum_{i=1}^{n} \xi_i$ may be less than unity.

seem to confuse the issue, in principle and in practice. Thus, in practice and for continuum one-way variables it would substitute a simple unique result by indefiniteness. For discrete variables, the a priori probabilities would replace the moderate uncertainty, $w/(\prod_i a_i)$, in (2.7) and (5.22). The result would be to blow up the uncertainty if not to distort the issue completely. In other cases, an a priori probability may mask a lack of existence of probability.

Concluding remarks

In most of the topics and in each chapter of this paper there is an implicit, if not explicit, connection to Brownian motion. Vibeke Nielsen and I have studied Brownian motion of Hamiltonian systems, partly as a further elucidation of the above considerations, and partly on its own merits. We intend to publish the results in a separate paper. In connection with the present work I want to express my great indebtedness to Vibeke Nielsen for numerous discussions and penetrating criticism.

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References

1) TH. BAYES: An Essay towards Solving a Problem in the Doctrine of Chances. Philosophical Transactions **53**, 376 (1763), **54**, 298 (1764); Ostwald's Klassiker der exakten Wissenschaften, Nr. 169 (1908).
2) L. BRILLOUIN: Physical Entropy and Information II. J. Appl. Phys. **22**, 338 (1951).
3) H. B. G. CASIMIR: On Onsager's Principle of Microscopic Reversibility. Rev. Mod. Phys. **17**, 343 (1945).
4) S. CHANDRASEKHAR: Stochastic Problems in Physics and Astronomy. Rev. Mod. Phys. **15**, 1 (1943).
5) R. T. COX: Probability, Frequency and Reasonable Expectation. Am. J. Phys. **14**, 1 (1946).
6) H. CRAMÉR: Mathematical Methods of Statistics. Princeton University Press, (1946).
7) J. L. DOOB: Stochastic Processes. John Wiley, New York, (1953).
8) R. A. FISHER: Statistical Methods and Scientific Inference. Oliver and Boyd, Edinburgh & London, (1956); cf. also: Contributions to Mathematical Statistics, John Wiley, New York, (1950).
9) E. T. JAYNES: Information Theory and Statistical Mechanics. Page 181 *in* Statistical Physics, Vol. 3. W. A. Benjamin Inc., New York, (1963).
10) H. JEFFREYS: Theory of Probability. Clarendon Press, Oxford, (1961).
11) A. KATZ: Principles of Statistical Mechanics: The Information Theory Approach. Freeman and Co., San Francisco, (1967).
12) J. LINDHARD & VIBEKE NIELSEN: Studies in Statistical Dynamics. Mat. Fys. Medd. Dan. Vid. Selsk. **38**, No. 9 (1971). In the text, this paper is referred to as SSD.
13) J. LINDHARD: Influence of Crystal Lattice on Motion of Energetic Charged Particles. Mat. Fys. Medd. Dan. Vid. Selsk. **34**, no. 14 (1965).
14) D. V. LINDLEY: Introduction to Probability and Statistics from a Bayesian Viewpoint, I, II. Cambridge University Press, (1965).
15) L. ONSAGER: Reciprocal Relations in Irreversible Processes, I. Phys. Rev. **37**, 405 (1931); II, ibid. **38**, 2265 (1931).
16) J. S. ROWLINSON: Probability, Information and Entropy. Nature **225**, 1196 (1970).
17) C. E. SHANNON & W. WEAVER: The Mathematical Theory of Communication. University of Illinois Press, (1949).

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