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(recevuto il 16 Giugno 1971)

Summary. — We discuss the conceptual problem of understanding irreversibility and the arrow of time. We point out that by generalizing the concepts of system and state, and the mechanics which governs them, it is possible to create the conceptual framework in which the occurrence of irreversibility can be understood naturally. The destruction of correlations is the principal mechanism which, in the generalized evolution given by a stochastic dynamics, leads to the increase of entropy and all the consequences of the second law. In the Appendix, we treat the case of two interacting spin systems and show that the destruction of correlations and the appropriate stochastic dynamics lead to irreversibility.

1. — Introduction.

MAXWELL (*) dealt with mechanics and thermodynamics in his original formulation of kinetic theory. BOLTZMANN (**) generalized Maxwell's results, advanced a new definition of entropy and sought an explanation of thermodynamic behavior on the basis of the fundamental equations of mechanics. BOLTZMANN had raised very important questions, and had gone a long way

(**) L. BOLTZMANN: Wien Ber., 53, 195 (1886); 63, 337 (1871); 66, 276 (1872); Lectures on Gas Theory, 1899-1908, English translation by S. G. BRUSH (Los Angeles, 1964).
in answering them. In the course of time, other people (*) said more and more clever things about Boltzmann's work, and soon enough the whole field became rather murky. It has seemed to us that the current situation in statistical mechanics, especially in the treatment of irreversibility, is rather confused in its conceptual structure and mathematical formulation. It is our impression that many people working in this field are unwilling to ask the original questions and to discuss the fundamental concepts relating to the origin of irreversibility.

In this paper we re-examine some of these original questions and the conceptual basis of the nature and increase of entropy, irreversibility and the arrow of time. In the following Sections we discuss certain enlargements of the concepts of the thermodynamic system, its state and its dynamics. The mechanism of the destruction of correlations in a generalized dynamics provides the natural law which explains irreversibility. In the Appendix, we give an outline of the mathematical steps of the generalized dynamics, and give an illustrative example of how the destruction of correlations as a natural law produces irreversibility.

2. – The statistical system.

In classical theory the entropy was originally associated only with stationary thermodynamic states, that is states in thermal equilibrium. There the entropy is considered as a state function, the state being defined by a certain temperature, pressure and other macroscopic variables. In equilibrium thermodynamics one can always define the entropy of a many-particle system, where the number of particles becomes arbitrarily large, even infinite. This device, the taking of the so-called thermodynamic limit, in the deeper sense is somewhat mysterious. If the attitude is taken that the entropy is not defined unless an infinite system is considered, then of course it is only a special system that is being considered, and not just any physical system. However, we would like to have theories that describe phenomena that we actually see, even though the necessary idealization is made from experience. In mechanics, for instance, we idealize the situation and say that a body on which no external forces act shall continue in its state of rest or motion. The idealization is made from experience in order to talk about a particular finite system. The purpose of idealization is to replace

an infinite, open, complicated system by means of a simpler system that we can interpret.

The idealization used in statistical mechanics, with appeal to the thermodynamic limit, seems to go in the opposite direction. What we should deal with is a finite system, and we should demonstrate that its entropy increases. In the thermodynamic limit, we seem to have an ideal system with an infinite number of objects, in an infinite volume, but a constant density. It is neither sufficient nor relevant to talk about special things related to the pressure, semi-permeable membranes, osmosis and the thermodynamic limit. In the laboratory we deal with finite systems, with the thermodynamics of finite systems, and we must define all the quantities we make use of. It is not quite legitimate to talk about a system having hidden regularities or hidden conserved quantities which can be explored by analysis. We need a version of statistical mechanics in which finite systems are dealt with, the entropy is defined for all configurations at all times, and there exists a mechanism for witnessing (or describing) the increase of entropy of the system. The important thing is to build the relevant mathematical, dynamical model; the model obviously must change depending upon the features of the experiments that have to be explained. It is the entropy of a finite physical system that appears to increase, and we must have a suitable dynamical model of such a system that would show this characteristic.

Statistical mechanics attempts to describe a macroscopic system in terms of its microscopic constituents. In the description of the system, we do not deal either with macroscopic or microscopic dynamics. The taking of the thermodynamic limit is justified by saying that the number of atoms or molecules in the system is very large.

We should clearly recognize that, if the averaging comes about only when the number of atoms or molecules is infinite, and not just very large, and if the increase of entropy comes about in the limit of an infinite number of particles, then the whole procedure has nothing to do with physics. If it is claimed that the thermodynamic limit is taken for “simplicity,” then it must be made clear for what. Is the purpose of taking this limit the ease of calculation? Or, is its purpose to give meaning to certain basic quantities (*)? If the purpose of the limit is the convenience of calculation, one would have to accept that as the reason—but we have to know why certain things are being done, and verify that the mathematical phenomena in the limit are not different in character from what actually happens in Nature.

Suppose a system consists of one or one hundred atoms. Is it, in either case, a thermodynamic system? Can it be regarded as a model of a statistical system? Could it approximate a thermodynamic system in experiments?

(*) For instance, the phase is not defined in the theory of phase transitions until the thermodynamic limit in infinite volume is taken.

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Most people would answer "no", but the "no" should not be accepted with
finality. Indeed, it may be quite difficult to make calculations when, say, ten
or a hundred particles are involved. We know that there are all kinds of
difficulties in computing things in the three-body problem; to deal with a hundred
particles in a mechanical theory would be very difficult indeed. The question
really is whether in statistical mechanics it is the difficulty of calculation with
a finite number of particles (however large this number) that necessitates the
taking of the thermodynamic limit, or the number of particles has to be infinite
for statistical mechanics to be applicable (*)).

Again, we ask whether the concepts like "averaging", "randomness",
"ergodicity", etc., are employed as a means for effecting an ease of calculation,
or whether they are really intended to produce (or understand) irreversibility.

Clearly, integration is much easier than summing up over a very large
number of terms, and in many approximations we would rather perform the
integration than the summation. However, we must remember that if the
sum of the quantities considered is not infinite, the integral should also not be
infinite. If the integral exhibits some peculiar features, then we should ask
where and why we picked up these features.

It is, of course, quite possible that under the conditions in which the models
of statistical mechanics are legitimate, the statistical mechanics of ten particles
will not be as satisfactory as that of ten thousand particles, and certainly
not as satisfactory as that of a still larger number of particles, almost
approaching infinity.

In most cases, however, when use is made of an infinite number of particles,
the character and goal of the original physical problem are changed or lost.
As a consequence of this, one has to appeal to "ergodic" properties, "irregular"
constants of motion, "space-filling" curves, etc. This should not be necessary.

(*) The thermodynamic limit, at times, may be a useful idealization so long as one
realizes that it does not really exist. The gravitational and electromagnetic forces
make it impossible to use a real thermodynamic limit. It is true that, with certain obvious
modifications, two liters of hydrogen behave as one liter of hydrogen, but if we put
together $10^{45}$ liters of hydrogen, the gravitational forces will change the situation entirely.
There will be other problems even if one disregards gravitational forces.

When correlation exist—one-particle, two-particle, three-particle correlations, etc.—
they go on to higher and still higher orders, until they go to infinity in the thermo-
dynamic limit. Now there are systems in which only two-particle correlations are
important. It depends on how large the system is, even though finite, and how one
treats it. One can have thermodynamics also for a system of very few particles, and
in statistical mechanics one can have phase space for just a few particles, enabling one
to calculate all sorts of properties. In equilibrium thermodynamics, which can be con-
structed for a few particles or even one particle, the measurement can be made over
a finite interval of time and it causes no problems. This is not so in nonequilibrium
thermodynamics, because of the presence of correlations among other things.

Going to the thermodynamic limit is therefore a self-contradictory statement, but
many people do not seem to take this into account.
The question can legitimately be asked: "Is it possible to talk about the statistical mechanics of ten particles?" Indeed, it should be possible to do so, just as it should be possible to talk about the statistical mechanics of ten million particles. In fact, it is possible to talk about the statistical mechanics of a single particle. Very often we do just that, as when we talk about the thermal distribution of a single oscillator.

3. -- State of the system.

Let us consider a system of particles. What are the states of this system? The state of a classical system has often been defined by giving values for the positions and velocities of the particles. However, it is logically not really necessary to define the state in this way. A more general definition of the state of a system is that it describes a dynamical condition which associates suitable numerical values with all functions of the basic dynamical variables p's and q's in such a manner that linearity and positivity are maintained. It then follows that states with definite values of p and q (that is, the old states) are, in the new definition, the extremal elements of the convex set of generalized states. In this way, we shall obtain a series of symbols denoting these mappings of dynamical variables on which we can operate.

A dynamical variable such as \( f(p, q) \) is an abstract object. It is a series of symbols, and manipulations can be made between them. These symbols have equations of motion which tell us how the symbols change. And, what is a state? A state is a means of assigning numbers to the dynamical variables. A state is a particular assignment—an explicit and concrete assignment of numbers to all given dynamical variables. If we take this point of view, then assigning numerical values \((p', q')\) to \((p, q)\) and therefore assigning the numerical value \( f(p', q') \) to the dynamical variable \( f(p, q) \) is obtained by substituting the values of \( p, q \); it is one of the simpler ways of defining a state:

\[
\Omega(f(p, q)) = f(p', q').
\]

The more general statement is that in mapping of the algebras generated by \( p \) and \( q \) onto sets of numbers, certain properties would have to be satisfied. For example, one would want that the dynamical variable which is the sum of two dynamical variables be assigned a numerical value which is the sum of the values assigned to these two dynamical variables:

\[
\Omega(a_1 f_1 + a_2 f_2) = a_1 \Omega(f_1) + a_2 \Omega(f_2).
\]

However, it may not necessarily be required that the product of two values be represented by the product of their expectation values, that is,

\[
\Omega(f_1 f_2) \neq \Omega(f_1)\Omega(f_2).
\]
This is not an unusual requirement, because quantum mechanics has shown that products of operators need not necessarily have assigned values which are the products of their respective expectation values. There is also no logical reason why the two sides in eq. (3) should be equal at all. From these considerations, the definition of the state emerges as a rule for mapping of the algebras generated by the dynamical variables onto sets of numbers (*). Mathematically, we may write

\[ \int f(x, y)g(y)\,dx\,dy = \Omega(f(y, q)) \]

with

\[ \int g(x, y)\,dx\,dy = 1 \quad \text{and} \quad g > 0 \]

(\(g\) being nonnegative and normalized).

The state is the ensemble associated with the distribution \(g\). To say that the state is described by an ensemble is not to be construed as ignorance on the part of the physicist; it is an ensemble, and the distribution \(g(x, y)\) characterizes the ensemble. The ensemble is a state which is described by a rule for mapping, and \(g\) is its characteristic distribution; it is obtained by giving a rule for mapping functions onto numbers.

A state for a linear ensemble is a convex set, in the sense that the weighted positive average of a series of states is also a state (†). For instance, one could take the sum of the two states divided by two. This would be a new state for the system, and it would have the property that we could map numbers onto themselves because a number is also a dynamical variable. A convex set is the set of all normalized linear combinations of its extremal elements. A point which cannot be expressed as a normalized linear combination of any pair of elements is called an extremal point; it lies on the boundary, but the set of these extremal points may not coincide with the boundary (‡).

4. – Notions of ensemble and temperature.

In order to deal with a physical system it is necessary to define the notions of enclosure, temperature and interaction with the outside. These cannot be obtained from the consideration of a given particle. A single particle does not necessarily have a temperature, and one might even say that ten million particles by themselves do not necessarily have a temperature. For instance, if

(‡) In the case of a circle, all points on the boundary are external points, while, in the case of a triangle, only the vertices are external points.
we have a collection of particles in a perfectly reflecting cavity, which is a legitimate mechanical system, it is claimed that this system has a temperature. We maintain that it will never really have any temperature. That does not mean that the temperature is zero or something else, but rather that it does not have the property called temperature. The state of motion which the system starts out with shall continue forever, and it has just that state of motion; one ought not be convinced to the contrary by someone who produces a very-well-defined existence theorem which shows that there are dynamical systems for which the situation is ergodic or quasi-ergodic. We are interested in actual physical systems before us, and our statements have to be true for simple systems in conventional containers no less than for mathematically esoteric ones. In actual experience, we find that all mechanical material systems approach equilibrium, not just those which are governed by some peculiar Hamiltonian; we should not be content with having to find peculiar varieties of Hamiltonians that lead to the thermodynamic equilibrium of certain especially chosen systems.

Now let us consider the notion of temperature. Temperature cannot be defined for a system of particles which are always in pure states. Temperature exists only for those states which are described by a suitable density in phase space. These are different kinds of states of the systems, but then we are called upon to describe new (other than merely mechanical) phenomena. We ought not look for the thermodynamic variables like temperature in the large number of degrees of freedom of many particles or in a particular Hamiltonian. When we wish to extend our physics, we must concomitantly adjust to it by introducing new concepts and enlarging our set of dimensions (*). We should look for the explanation of thermodynamic behavior on the basis of the new kind of statistical state, the generalized state, that we define.

Temperature is not attributable to any « pure » state, and it is therefore not related to conventional mechanical variables. Temperature is not a mechanical variable even though it is defined for a mechanical system.

In fact, temperature is the modulus of a distribution (**). Consider, for instance, Maxwell’s distribution of velocities for a nonrelativistic particle (mass $m$)

\[
\frac{N_v dv}{N} = \frac{4}{\sqrt{\pi (\beta m)^2}} v^2 \exp \left[ -\frac{\beta}{2} m v^2 \right] dv \quad (\beta = \frac{1}{kT}).
\]

(*) For example, once we used to be limited only to the use of positive energies, temperatures and probabilities. Nowadays we have less difficulty in adjusting to these ideas because of our vastly extended physical picture (*).

(**) For instance, we take note of such concepts as the negative entropy, negative temperature and negative probability.

This distribution gives the fraction of molecules which have speeds between \( v \) and \( v + dv \). All of these particles have, of course, well-defined velocities. The Maxwellian distribution becomes more and more accurately realized when the number of molecules becomes larger and larger, and ultimately tends to infinity.

An ensemble in Gibbs' method consists in making many mental copies of the physical system. Each member of this set corresponds to a well-defined point in phase space. The distribution of these phase points is given by a probability function in phase space such that the fraction of occurrence of the members of this set lying in any volume of phase space is proportional to the volume multiplied by the density. This device was necessary because the concept of the state was reserved for only the pure states. In fact, however, this construction gives the actual physical state as a rule for mapping in the same way as the definition of an arbitrary state in eq. (4). The pure state may now be considered as the extremal elements of this set. Thus the ensemble itself now becomes an element of the convex set, and we have only one system whose states are more general than assumed previously. In Gibbs' method, we make mental copies of the same physical system, and we can make as many copies as we want; the Maxwellian distribution describes the fraction of these mental copies. This method is therefore not limited by the number of molecules—we may consider a few or even a single molecule. Thus, it is not real or unrealistic to think of a single degree of freedom for the discussion of statistical states; in fact, we do actually do so, as in the derivation of Planck's law by the method of Bose, obtaining for the average energy of the single mode th expression

\[
E_n = \frac{\hbar \nu}{\exp [\hbar \nu/kT] - 1}. 
\]

In Bose's method, it is the levels or excited states of a single mode of the radiation that are dealt with (*). While accepting Gibbs' prescription, we can go further in the generalization of his abstraction.

We can deal with statistical states and their distributions; the latter as in fact the coefficients of the decomposition of the state as a linear combination of the extremal elements, a quantity which may itself be computed from general principles. The Maxwell and Planck-Bose distribution functions, eqs. (5) and (6) respectively, are special examples of these states. That is, the Maxwellian distribution would be treated as Gibbs would treat it, with the recognition that it is the ensemble itself which is the state, and not that it is an ensemble of states.

(*): Here the energy distribution to the mode is given by the electromagnetic energy per unit volume \( E = (8\pi^2/c^3)E_n \).
That is, this linear combination itself is defined as a state (\(^1\)). And, the temperature is a characterization of this distribution or density function of the ensemble. The characterization of the temperature depends upon the nature of the Hamiltonian. Not every distribution has a temperature; the extremal elements do not indeed have any temperature. The temperature is the property of a class of distributions, and not of any mechanical state.

Let us pursue further the connection between the temperature and the ensemble. Consider a single particle at a certain temperature. Normally, this consideration does not make sense, because one wonders what is meant by the temperature of a single particle which has well-defined position and momentum. Of course, we will have to endow the particle with the necessary properties in order to describe a new conceptual situation. If single particles are just those things which have well-defined positions and momenta, then these particles are clearly unable to describe a system at a certain temperature. Of course, we can give these objects some other name, although they will still be described by \(p\)'s and \(q\)'s and their equations of motion, but they will not be particles in the conventional sense with certain prescribed states. The question we ask is this: What is the generalized state of a particle (the new object) with temperature?\(^1\)

We assert that the particle with temperature will no longer be represented by an extremal state, although it will still be represented by a state which maps \(p\)'s and \(q\)'s, and functions of \(p\)'s and \(q\)'s, in such a way that we would get Maxwell's velocity distribution for a collection of particles. That is, for any function \(f(p, q)\), we define a state at a certain temperature \(T\), or inverse temperature \(\beta\), by requiring that the expectation value of the function \(f(p, q)\) be mapped according to the rule

\[
\langle f(p, q) \rangle = \frac{\int f(p, q) \exp \left[-\beta H(p, q)\right] dp dq}{\int \exp \left[-\beta H(p, q)\right] dp dq}.
\]

This is the state of the system which is now considered as a single particle. Now if we have ten particles, identical in the Maxwellian sense, all we need to do is simply to multiply this quantity by ten in order to calculate the appropriate dynamical quantities of the system such as its total energy, total momentum, or total angular momentum. Thus, it is not the averaging of this quantity over various states; it is actually the computation of its value for that particular state. It is of course true that such a state—the statistical, stochastic, probabilistic, extended, or generalized state—can be expressed as a linear combination of pure states. We just say that this is the state of the

\(^{(*)}\) Each velocity or state with any velocity is a pure state corresponding to an extremal point, but a probability distribution over them is a linear combination of these states.
system, although it is possible to expand this state in terms of other pure states (*)

As we have mentioned earlier, it is not possible to introduce temperature in a mechanical system, because the temperature is related to the impurity of the states—that is, the states must not be distinguished extremal elements of the convex set, but must lie within the extremal elements among a special class of states.

5. – Approach to equilibrium.

Our experience is that all material, mechanical systems approach thermodynamic equilibrium, not just those that are governed by some peculiar Hamiltonian. How does a system approach equilibrium?

As we have defined it, the system has all the states and we can talk about a continuous transition from one state to another. The taking of some magical limit (such as an infinite number of particles, large volume, etc.) or some average that results in the increase of entropy should not be considered satisfactory. The mathematical model ought to be such that one can actually calculate the entropy and discuss the evolution of the system.

In the process of collision some exchange of energy and momentum takes place between various particles. If the initial condition of the particles was such that their relative velocities were uncorrelated with their positions, then at the end of collision correlations are established. In his classic treatment, Boltzmann (†) decided that, after collision, the resulting correlations may be neglected, and by doing this at the end of every collision process Boltzmann was able to show that a quantity $H$ for the system decreases, while the entropy $S$ increases, signifying the decrease of order.

This is essentially the dynamics of the system which Boltzmann considers. The system initially has certain distributions, and the dynamics consists of two steps: one step in which there is a collision, and the second in which the correlation generated by the collision is destroyed. This is the source of the increase in entropy, the increase of entropy being, not in the collision, but in

(*) For instance, given a function $f(x)$, which is integrable in the interval 0 to 1, or $-1$ to 1, we can expand it in terms of the standard polynomials with coefficients. We do not say that the only true functions are the standard polynomials. We have the coefficients of expansion, and we are interested in describing all functions. Similarly, we are interested in describing all states. Thus our mechanical system is more general; it is richer than the mechanical system usually defined. It is a new entity, and if one does not like to call it a "particle" one may call it something else. But we maintain that the dynamical model of the thermodynamic system is in fact just this entity, and nothing else.
the destruction of correlation. And this process is irreversible because something
is being destroyed and not created. The collision process itself is completely
reversible. However, this treatment cannot be considered as a derivation of the
increase of entropy from the equations of mechanics, because mechanics does
not ask one to destroy the correlations. The responsibility for doing the latter
must lie outside the Hamiltonian law.

The question still remains: Does the entropy of a system increase? In
terms of the physical experiment, it obviously does. For instance, ice melts,
and the entropy increases. Does the entropy of the system, defined in terms
of the Hamiltonian mechanical model with all its collisions, etc., increase? The
answer is no. It would increase only if the mathematical model were also to
include the step of destroying the correlations. But if the correlations are
deliberately and systematically destroyed, the model is no longer Hamiltonian.

The suitable mathematical model that would be necessary would perhaps
be one for an enclosure whose walls are maintained at a particular temperature,
one which would have no other interference. The surface of the enclosure, itself
considered as a dynamical system, would be in some statistical state, undergoing
some thermal vibrations, as a consequence of which perhaps certain correlations
are destroyed. It is clear that because of the need for the destruction of cor-
relations, something unmechanical of necessity would have to be introduced
into the mechanics of the model of the system (*)

In fact, as we have stated earlier, we do not need to take any limits or to
consider any esoteric systems. We can take ten particles or even a single particle
and should be able to demonstrate the increase of entropy. Often there are
other systems, not particles, which collide—such as spin systems (ferro-
magnets), collection of harmonic oscillators coupled to each other—in which
also we should be able to demonstrate the increase of entropy. A coupled system,
for instance, evolves in a certain manner for a time, and at the end of that time

(*) There have been numerous attempts to understand the increase of entropy and the
nature of irreversibility, however, our own conviction that the explanation of these
must lie in the introduction of something essentially nonmechanical (albeit so small)
in the mechanics of the system, reminds us of Elijah’s experience on Mount Horeb (*).
In Boltzmann’s work, for instance, there is a “huge” system of $10^{24}$ or $10^{25}$ particles,
with the lightning and thunder of the collisions and correlations between particles—but
the increase in entropy is not in it. There is summation over a large number of collisions,
but the increase of entropy is not in it. Then comes the sound of a gentle whisper—
which asks that the large numbers of correlations be quietly dropped. With Boltz-
mann, we cover our face and say that the entropy has increased! However, by talking
about infinite numbers of particles for which the differential equations are not defined,
and that therefore ergodic or quasi-ergodic processes have to be considered or thermo-
dynamic limit taken—by all these things, by giving the problem new names, the funda-
mental confusion is perpetuated and the problem is not really solved.

(*) The Holy Bible, King James Version, The First Book of Kings, Chap. 19,
Verses 11-13.
the correlations between the components are destroyed; by doing the experiment it is actually possible to show that the entropy of the system has increased.

6. Generalized state for the statistical system.

In order to make a mechanical model of a thermodynamic system, we must enlarge the concept of a state. Instead of having «pure» states, or states designated by extremal points, we could have states which belong near the boundary rather than inside the convex set. The «pure» states come as a special case, and it is not necessary to specify whether classical, quantum, or any other algebra is being used, but they are extremal in the sense that every state of the system can be expressed as a probability average, i.e., normalized positive linear sum, of these states. In quantum mechanics the pure states are the extremal points (or distinguished boundaries) of the convex set. Also, in discussing quantum states, we have to deal with density matrices rather than state vectors. In the same manner as one can extend the notions of mechanics to the other phenomena of physics, we can generalize the dynamical equations from describing particles alone to describing other things. Just as we generalize the notion of dynamics from describing motion to describing any change, we can generalize the notion of an ensemble.

In Gibbs' method the device of constructing an ensemble was necessary because the concept of the state was reserved for only «pure» states. As we have noted earlier, this construction gives the actual physical state as a rule for mapping as the definition of an arbitrary state, the «pure» states being considered as the extremal elements of the convex set, and the ensemble itself becoming an element of the set. So that we now have only one system, which has more general states than assumed previously. With this new definition, it is conceivable to talk about a dynamics which would change the «purity» of the state, which would move one of the extremal states to states which are inside the allowable set of states. When this is done, the phase-space densities are no longer matters of «ignorance»; they are statements about the «knowledge» of the state of a physical system.

Now we maintain that a system which only has the conventional Hamiltonian equations as its internal dynamics cannot approach equilibrium, because, in the evolution of such a system, pure states evolve into other pure states and it cannot be otherwise. Even if we start out with statistical states, the patch in phase space may evolve into a patch of the same extent, so that the amount of impurity (or purity) of the state is not altered. Especially if we start out with «pure» values of $p$'s and $q$'s, the state is represented by a single point in phase space and it will go to another point in phase space; there is just no question of its extending itself into anything else. If it is required that in its evolution the purity of a state of the system be preserved, then Hamiltonian
some reflections on the nature of entropy, irreversibility etc.

dynamics is fine, but if the statistical evolution of the system is to be considered, then a more general dynamics is necessary. There is no law which predetermines that the equations of motion be such that $p$ and $q$ develop in a certain manner. Of course, when ordinarily one talks about a collection of particles, one understands by the dynamics of this system that a particular set of the values of $p$'s and $q$'s changes into another set of values, because there exist differential equations (Hamilton's equations) for them. Purity of the state is an intrinsic attribute with respect to Hamiltonian dynamics, but a variable attribute with respect to the generalized stochastic dynamics necessary for the statistical evolution of a system; in the latter case purity ceases to be an intrinsic parameter, and no quantity remains constant.

The physical system, which we consider, is defined more generally. It is described by a state, and the dynamics describes the change in the state of the system without changing the essential nature and intrinsic properties of the system, thus its mass or the number of degrees of freedom will remain unchanged. Auxiliary or external characteristics may alter, and their change or variability in the course of time constitutes motion. This is precisely what we mean by the evolution of the system: the intrinsic nature of the system remains unchanged, but its accidental characteristics, initial values, or specifications may change.

From this point of view dynamics, in the more general sense, is a statement about the evolution of the system, a statement about the change of status of the system. Dynamics gives the evolution of the status. With this viewpoint, it does not consist in giving a set of differential equations describing the evolution of $p$'s and $q$'s, but rather in a statement about the development of the distribution function. If by mechanics one understands only collisions between particles given by a Hamiltonian, then mechanics can never lead to thermal equilibrium; the Hamiltonian equations of this mechanics, on integration, would take the system from one pure state to another pure state. Our dynamics has to be more general than that (*).

(*) Consider, for example, the density matrix of a 2-level system given by the Bloch equation

$$
\rho(t) = \frac{1}{2} (1 + \sigma \cdot \mathbf{P}(t)).
$$

Any Hamiltonian evolution will now preserve the square of the polarization vector (i.e. the magnitude of polarization) given by

$$
P_1^2 + P_2^2 + P_3^2 = \text{const}
$$

(independent of $t$ for any Hamiltonian).

The only requirement on the polarization vector is

$$
P_1^2 + P_2^2 + P_3^2 < 1,
$$

and the equality corresponds to the pure or extremal state of the density matrix. The convex set of states in this case may be identified with the sphere of unit radius in
If we define a state by assigning values to $p$ and $q$, then the Hamiltonian equations take this state into another pure state, however we can define a generalized state by means of a collection of pure states and their probabilities. A linear combination of pure states with suitable positive coefficients can rep-
three dimensions. The set of extremal elements or points coincides with the two-dimensional surface of the sphere. Any Hamiltonian evolution is therefore a rotation of the sphere into itself.

In stochastic dynamics, on the other hand, a state represented by an extremal point may move to a point in the interior of the sphere, and a point in the interior of the sphere would move as determined by linearity. An example of this given by the Bloch equations

$$P_3 = \frac{P_2 - P_3}{T_1}$$

and

$$P_1 + iP_2 = -\frac{P_1 + iP_2}{T_1} - i\omega (P_1 + iP_2),$$

where $T_1$ and $T_2$ are the longitudinal and transverse relaxation times. There is no Hamiltonian which would yield this.

What is the possible relation of the Bloch equation to the Hamiltonian scheme? Any Hamiltonian which will give rise to a change in the polarizations would induce correlations between the longitudinal and transverse components. Any Hamiltonian which will cause a change in the longitudinal component $P_3$ will establish a correlation between the longitudinal and one or both of the transverse components. Such a correlation term is missing on the right-hand side of the Bloch equation (11), i.e. $P_3$ does not depend on $P_1$ and $P_2$. Thus, we are led to look for the origins of stochastic dynamics in the destruction of correlations. The argument which we are constantly seeking to enforce in this paper is that the increase of entropy, irreversibility and the origin of stochastic dynamical behavior, indeed the existence of nonequilibrium thermodynamics, lie in the loss or destruction of correlations (**).

Thermodynamics is only possible and indeed inevitable, when we discuss the behavior of a limited part of an unlimited universe. Thermodynamics of the universe as a closed system, as such, does not make sense, because what we always deal with is a finite system as a part of the larger universe. In spite of its generality, thermodynamics is a manifestation of the essential inadequacy of our description of the unknowable universe at one and the same time. The universe itself is the one physical system in which there is no distinction between initial condition and laws (*)

Just as Mach maintained that inertia arises on account of the existence of distant matter, we maintain that the thermodynamic equivalent of distant matter is the external universe, and the equivalent of inertia is the loss of correlations. What is being constantly propelled in the universal thermodynamic wind is the nonequilibrium thermodynamic evolution of a subsystem by means of the loss of correlations. The latter exists in nature, just as inertia exists, and our thermodynamic model must reflect this as the basis of the dynamics of the system. What Boltzmann did was an admirable first effort in this direction.

(**) *Ignorance is the root of all decadence*, Nagārjuna.

(*) H. Bondi: Cosmology.
resent any general state of the system. Under a Hamiltonian evolution such a state would go into a linear combination of the transform of these extremal states with the same coefficients. Therefore, if the system does not correspond to a thermal state (i.e. a state with temperature), then under the Hamiltonian evolution it would never evolve into one.

The evolution of a state is linear in the sense that the state evolves, the probabilistic combination of states evolving to the corresponding probabilistic combination of evolved states. Thus, if each pure state is defined by a value of $p$ and $q$, i.e. a point in $T$-space or phase space, then this point goes into another point. The probabilities themselves remain unchanged for each pure component; its location may change, but the purity of the state remains unaltered. Hence, the entropy cannot increase, because the entropy is essentially a function only of the purity of the state.

What then is an equilibrium state? It is the state associated with the maximum entropy at a certain configuration, subject to the constraints that the total number of particles, total momentum and energy, etc., are fixed. The state which corresponds to this situation is unique, and for classical particles it leads to the Maxwell-Boltzmann distribution, that is, a well-defined state.

What is the state of a system which has a certain temperature? It is an impure state, and the impurity is governed by essentially the Maxwell-Boltzmann distribution, this being true of each particle, independently of all other particles. It is a very impure state, and no matter where we start we must arrive at this state as long as the total energy is fixed. An evolution of the system leading to a thermal state is not attainable for the Hamiltonian system, because the latter preserves the purity of the state. From classical Hamiltonian mechanics, therefore, we cannot arrive at an equilibrium state in the thermodynamic sense. The specification of pure states requires only one point in phase space, although this point is given by assigning numbers to a whole lot of parameters characterizing the state. For impure states, we have to specify a distribution in phase space. In the special case of the state of a system at a fixed temperature, we need only one parameter, which can be $T$ or $\beta$ ($=1/kT$).

Thus, it is clear that, for the description of thermal states, we need a patch or distribution in phase space. The evolution of the state is not displacement of a phase point to another point, but as it moves the point or the patch should expand. This cannot be done by Hamiltonian mechanics, as we have insisted several times, because Hamiltonian mechanics views the evolution of $p$ and $q$ as a function of the previous $p$ and $q$. All this has nothing to do with quantum mechanics, because in quantum mechanics the $p$'s and $q$'s are not specifically defined for defining a state. It has also nothing to do with quantum-mechanical uncertainty, because the uncertainty which is characteristic of quantum-mechanical measurement is also preserved in the time evolution of the system, just as the purity of a state is preserved.

There is just no point in introducing some other kind of uncertainty or lack
of precision in the definition of the state in order to obtain an approach to thermal equilibrium, because the introduction of such a device would itself become a constant of the evolution. The important thing is that the impurity of a state may grow if the approach to thermal equilibrium is to be realized. For this evolution, extremal states must move inward, from states of some impurity to states of greater impurity; the latter must be the case for an increase of entropy to occur.

What we have said amounts to the following: 1) we must enlarge the notion of dynamics, make the dynamical model richer and let it exhibit more characteristics; 2) we cannot introduce temperature unless we are prepared to consider laws of evolution which would alter the purity of the state of the system.

7. – Conventional formulation of generalized mechanics.

7.1. Boltzmann's method. – BOLTZMANN derived his collision equation and H-theorem as follows. He considered a dilute gas, dilute enough for three-body and higher-order collisions to be neglected. He then assumed that at a chosen instant the gas, although homogeneous in position (co-ordinate space), has a certain velocity distribution. The effect of the collisions then is to change the marginal distribution function in velocity, and this change is embodied in the Boltzmann equation

\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial r} + F \frac{\partial f}{\partial v}, \]

where \( f(r, v, t) \) is the distribution function and \( mF \) denotes the force on a molecule \( m \) at \( r, t \); \( r \) denotes the space co-ordinates, and \( t \) the time. This equation, which is true only at the preassigned instant when the space distribution of particles was uniform, that is, \( f(v, r, t) = f(v, t) \), is then assumed by Boltzmann to hold at all times. This leads to Boltzmann's H-theorem, which says that

\[ H(t) = \int f(v, t) \log f(v, t) \, dv \]

is a monotonically decreasing function of \( t \), leading to the monotonic increase of the entropy. This is a consequence of Boltzmann's equation, quite independent of the details of the collision function.

In terms of the state of the system, Boltzmann's description deals with a very special state of the gas, one in which there are no correlations between the positions and velocities of the particles (*). Moreover, there is no correlation

(*) BOLTZMANN treats his gas as a special fluid which is as far removed physically from a "nonturbulent" liquid as possible, because in the latter the velocity distribution is a well-defined function of the position, given by the liquid velocity at that point. In Boltzmann's model, there is no correlation between the velocity and the position, the two being totally independent. A turbulent liquid or a dense gas is something in between these two extremes.
between the velocities of the particles themselves, so that BOLTZMANN is able to write, for this special case, a single velocity distribution function for the entire gas instead of writing a distribution function of $n$ velocity vectors, $n$ being the number of particles. By this device, BOLTZMANN is able to describe the state of the gas at a chosen instant by means of this special velocity distribution function.

Now if we were to make use of a Hamiltonian law of evolution, such a given state of the gas would develop into a more complicated state (that is, not having the special properties assumed earlier) after one or several collisions. The gas will develop correlations of arbitrary complexity. BOLTZMANN, however, chose to invoke the hypothesis of molecular chaos and insisted that at any time, after any number of collisions, the state of the system should be describable again by the same special type of state assumed earlier—that is, by the single velocity distribution function. Let us call these states which are described by single velocity distribution functions as Boltzmann states. According to a Hamiltonian law of evolution, the system would not proceed from a Boltzmann state to a Boltzmann state. Next BOLTZMANN supplemented the Hamiltonian law of evolution by neglecting the correlations which are generated.

In Boltzmann’s treatment, a number of things were not clear, and the same things have seemed to perpetuate the confusion in the discussion of irreversibility and the increase of entropy. 1) BOLTZMANN neglected all correlations because he dealt with Boltzmann states only, and his equation was unable to deal with a situation of greater complexity; 2) BOLTZMANN neglected higher-order collision terms whose effect, although small to start with, might become considerable later on; 3) Boltzmann’s treatment of two-body collisions involving identical particles is already defective, since the indistinguishability of particles automatically implies a dependence of the collision probability on the distribution function for both the initial and final velocities of the colliding particles (*); 4) if we accept Boltzmann’s device of dealing with his special definition

(*) In Boltzmann’s case, the collision term is given by an integral over
\[
\{f(u_v)/f(u_{v'}) - f(u'_{v})/f(u'_{v'})\}
\]
(where the primed quantities are those after the collision), while the correct collision term, based on indistinguishability of the particles, is given by
\[
f(u_v)/f(u_{v'})\{1 \pm f(u'_v)\} \{1 \pm f(u'_{v'})\} - f(u'_{v})/f(u'_v)\{1 \pm f(u_{v'})\} \{1 \pm f(u_{v})\}
\]
From Boltzmann’s equation, equilibrium is obtained by setting the collision term equal to zero, and one obtains
\[
f(u_v)/f(u_{v}) = f(u'_{v})/f(u'_{v})
\]
log $f(v)$ must be linear in the conserved quantities, and under suitable specialization this leads to the celebrated Boltzmann distribution formula
\[
f(v) = \exp \left[ -\beta E_v \right]
\]
where $E_v$ is the energy associated with a particle of velocity $v$. The correct collision
of the state of the system (Boltzmann state) and its evolution, it is clear that
the entropy increases, and that there is a preferred direction of time (one in
which $H$ monotonically decreases and $S$ increases) leading to unambiguous irreversibility. In Boltzmann’s treatment, there is a well-defined evolution of the
state and a unique value of the $H$-function at each instant of time; the
monotonic decrease of $H$ is deterministic. There is no question of its decrease being
more probable than its increase at any time (’).

\[ \log g_{\nu} = \log \frac{f(v)}{1 \pm f(v)} , \]

which should be linear in the conserved quantities, and with the constraints necessary
to derive Boltzmann’s distributions, we obtain

\[ g_{\nu} = \exp \left( \mu - \beta E_{\nu} \right) \]

and

\[ f(v) = \frac{1}{\exp(\beta E_{\nu} - \mu) \pm 1} , \]

which gives us the derivation of the Bose-Einstein (the Fermi-Dirac) distribution law;
the upper sign is for the B-E and the lower sign for the F-D distribution.

(*) Comment on Boltzmann’s method. Boltzmann’s was the first, and indeed the most
significant attempt to create a stochastic dynamics. In our view, the principal defect
of Boltzmann’s method lies herein: Boltzmann starts with Hamiltonian dynamics and,
by a series of intermediate ‘unmechanical’ prescriptions, obtains the desired
evolution as seen in nature. In Boltzmann’s method and all subsequent work, one
starts out with a well-defined Hamiltonian, but introduces the non-Hamiltonian
element of neglecting some or all correlations. In this manner, the stochastic
dynamics is not unrelated to the microscopic Hamiltonian, but it is not a consequence
of this Hamiltonian alone. In the usual kinetic theories one calculates the irreversibility
parameters, such as the coefficients of thermal diffusion and viscosity, from the
Hamiltonian, but the existence of these irreversible processes is contrary to a
Hamiltonian law of evolution.

We maintain that for the explanation of statistical mechanical phenomena the law
of evolution is not Hamiltonian, and by creating a generalized dynamics which is essentially
non-Hamiltonian we can rid ourselves of all ad hoc intermediate assumptions. Thereby
we can also shed all the paradoxes that arise in connection with Boltzmann’s equation
and the $H$ theorem, as well as the presence of the ‘mechanical’ explanation of the
second law of thermodynamics.

Given a purely classical mechanical system, it is not possible to introduce temperature
into the system unless a non-Hamiltonian evolution is introduced into it and it arrives
at a Boltzmann state. It is only by defining the system in a more general manner
that the temperature can be introduced in it. If we can destroy the correlations present
in the system at any suitable point, then a temperature can be introduced into the system
because the system will evolve eventually to a state when $H$ can no longer decrease,
having reached a minimum value subject to the given constraints. The entropy thereby
increases to its maximum value, subject to the constraints, and that leads (depending
upon the kind of identity assumed for the particles) to a Bose-Einstein or Fermi-Dirac
distribution.
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Whenever we make the pretence of describing an irreversible situation by means of the formalism of reversible Hamiltonian mechanics, there is always some step employed deliberately or unconsciously which introduces the non-Hamiltonian characteristics. In Boltzmann's derivation of the increase of entropy, the correlations are deliberately ignored. His explanation of why they have to be ignored is not satisfactory (\(\ast\)). The correlations exist in Hamiltonian dynamics, whereas they must be destroyed and the initial conditions disregarded in order to consider the thermodynamic evolution of the system. If we assume initial conditions with correlations, then the Boltzmann theory cannot describe the evolution of the system. It cannot describe the evolution because we only say how many atoms are in a certain part of \(\mu\)-space, but we do not know where to find the other atoms by only knowing that certain atoms are in a given part of \(\mu\)-space. When it is sought to describe irreversible phenomena by means of the reversible equations of motion, it is the manner in which the initial conditions are assumed that is important (\(\ast\)\(\ast\)).

72. Thermal bath. — The law of evolution for a system could be something as simple as the assumption that the system is in contact with a thermal bath,

\(\ast\) It is interesting to note that the transition from three-dimensional space or six-dimensional \(\mu\)-space (Boltzmann space) to \(6N\)-dimensional \(\mathcal{P}\)-space (Gibbs space) brought about an enormous clarification, because it gave us some indication of how the correlations arise. The Bohr-Kramers-Blatter ideas were restricted to three-dimensional space, and as a result they could not even reproduce the energy principle. Sommerfeld then took up configuration space, and the same basic ideas worked beautifully there. It is again the correlations which can be represented in configuration space, whereas they cannot be represented in ordinary space, just the same way as the correlations cannot be represented or described in Boltzmann space, but can be represented in Gibbs space.

\(\ast\)\(\ast\) It is important to emphasize the difference between thermodynamic irreversibility and the violation of time-reversal invariance. Many people insist on the fact that the equilibrium second law of thermodynamics remains valid in spite of this irreversibility, that it does not affect it. It is actually true that what enters in the usual formulation of the second law for equilibrium is the Liouville theorem. Even if Liouville's theorem were not valid, one could find another theorem, because, after all, what is needed is only a density in phase space. Classical mechanics is time-reversal invariant, but the problem of irreversibility is not. The second law of thermodynamics is independent of time-reversal invariance or violation of time-reversal invariance. Conventional time-reversal invariance is not defined in a theory of irreversibility.

Time is the essential parameter that gives us irreversibility, and the increase of entropy must exist in time. Time-reversal invariance has, among other things, a consequence which shows that absolute time is irrelevant, because for every finite time, we can go back and bring it back to an earlier position somehow. Now if time-reversal invariance is not valid, it is quite possible to assume that there is an absolute time. Well, in a certain sense, for the expanding universe, there is. And it may affect events in small details. When we talk about variation of entropy with time, it is the variation of the entropy with time only in a given direction.

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such as the one that is usually considered in thermodynamics. We must recognize, however, that the thermal bath cannot itself be a Hamiltonian mechanical system. The postulation of the thermal bath is in itself the introduction of a stochastic, non-Hamiltonian device to bring about the approach to equilibrium, and anything that approaches equilibrium contains a stochastic element in its dynamical evolution. The thermal bath cannot be expressed in terms of the equations of motion if it is to be used for the purpose indicated.

The system interacts with the thermal bath which is maintained at a certain temperature. This is just what happens in Brownian motion, for instance. In this case, a particle suspended in a liquid is continually hit by some other particles or aggregates of molecules, and therefore its dynamics looks random. In Brownian motion we do not observe molecules; we observe something that is hit by molecules. If the motion of the observed particle looks random, it is because the dynamics to which it is subjected contains certain components which have a statistical evolution. Now, the system itself would remain unchanged if different mechanisms of exerting forces on the particle are introduced; the mechanism could be a thermal bath or a random electromagnetic field.

The important thing is that something external is imposed upon the system that introduces the random or stochastic element and changes the evolution of the system from purely dynamical to stochastic or statistical. This is equivalent to the statement that, if you have a purely mechanical system, completely isolated, then energy and momentum are conserved in normal manipulations. However, if a system is governed by external forces, then as long as the forces are not time dependent, the moments of its constituent parts will be altered but not their total energy. If the system, that is thus maintained externally, is also arranged such that its time evolution is described from outside, then we find that the energy can actually be gained or lost by the system. What happens to this energy? The question is really meaningless, because the system maintained externally is not a closed system; it is an open system, and the energy that went into it was brought from the outside. If we treat the external forces as part of the dynamical system, then the system will not be considered as being maintained externally and its evolution would depend on the forces; in this case, of course, we would have a measure of energy changes due to external forces which, together with the initial energy, will be conserved.

Hence, we have the choice of describing the system as mechanical, in which case the energy is conserved, or we can treat it as a simple, externally maintained system, but then energy and momentum are not conserved. We can have a system in which there is an external thermal bath which maintains the system, and if that is the case we cannot talk about the increase of entropy of the total system consisting of the thermal bath and the system under consideration.

Gibbs came very close to this point of view. He sought to justify replacing time averages by ensemble averages, but all that is not really necessary. We do not need time averages. We need a mechanical system whose condition
at a given instant is specified, because it is a thermodynamic system at that
instant. The exact time-averaging procedure would not alter the symmetry
characteristics of the system. Furthermore, the time averaging for an infinite
period cannot give us any information about the change of entropy, because by
the process of time averaging the time has been removed. If someone determines
that time averages are related to ensemble averages, well and good, however
this does not affect the considerations we are advancing (').

Now, in order to define the system it is not really necessary to have a con-
tainer. For instance, we can have for our system a collection of harmonic
oscillators which are located on certain sites. So, a containing is not neces-
sary. The system has something outside it, but whatever is inside is always
Hamiltonian.

73. Ergodicity and nonequilibrium statistical mechanics. — The ensemble,
as far as we know, is the best way to consider many systems together. Also,
if we consider an ensemble, we become independent in our calculations from
the quasi-ergodic hypothesis, and the taking of ensemble averages has also
nothing to do with ergodicity. The ensemble is a set of states with somewhat
different properties, and one usually calculates averages over certain properties
of the members of the ensemble (**).

(*) In quantum optics, for instance, we have the important observation that we do
not have to make use of the ergodic theorem which relates time averages to ensemble
averages. There one recognizes that the ensemble averages are the primary things.
In optics when something is measured and there is a certain amount of coherence, we
do not really say that many oscillations take place and that the measurement takes
a finite amount of time; all that may well be true, but is somewhat irrelevant. We
can make a model in which at each instant of time we have an ensemble. The uncer-
tainty which is characteristic of quantum mechanics has nothing to do with the un-
certainty characteristic of the increase of randomness connected with the increase of
entropy.

(**) The difficulty of the ergodic problem, that is the assumption that the time averages
and the ensemble averages are the same under certain conditions, was treated principally
by von Neumann, Birkhoff, Hopf, Koopman and Loinger. von Neumann, Birkhoff
and Koopman essentially proved that, under certain conditions (which are the condi-
tions of the quasi-ergodic hypothesis), a time average of a system and the ensemble
average are identical. Wigner has also proved this ('). It has also been proved recently
that the validity of the quasi-ergodic hypothesis is much smaller than was thought
before.

The difficulty is that ergodicity came about because of a lack of desire to understand
the ensemble as a new system. Ensemble is a model of a physical system, because one
can make another model by saying that the ensemble is the time average of the
system—and then one does not need the ergodic hypothesis. If one believes that the
ensemble is the time average of a physical system, then one does not have any problem
in this regard. Now, it is quite conceivable that this is not so, and that the time
If one pursues the ensemble average as a new model, then the ergodic hypothesis has about as much relevance as the aether. The initial idea was that the time average is assumed in a very short time and it is equal to the ensemble average. Boltzmann also made these remarks in relation to the problem of the recurrence cycle being of the order of the age of the universe (11).

If we consider two gases inside a container, one on the left side and the other on the right side, that are allowed to mix, the pressure establishes itself in a fraction of a second, but the diffusion (so that there is an equalization) and the approximation to the ensemble properties takes days or weeks. This shows that some properties adjust to the average much quicker than others, and there are certain properties, not easily measurable ones, which probably never reach an average. There may perhaps be other properties that we do not even know about, in the case of which the problem of irreversibility and ergodicity may be neither relevant nor answerable.

It has traditionally been argued that by considering some averaging procedure for the mechanical model of the thermodynamic system, it is possible to show that the system behaves in a certain manner; for instance, by defining the entropy at all times in terms of \( \int \log f dp dq \), and showing that it uniquely approaches a maximum by the averaging procedure. However, it is only possible when the averaging procedure is accompanied by some approximation operation. We maintain that any genuine averaging procedure cannot alter the symmetry characteristics of the system, and we shall discuss this question from general considerations elsewhere.

7.4. Some remarks on the formulation of generalized mechanics. - In both cases, i.e., Boltzmann's method and that of stochastic dynamics, the procedure is to consider a system, let it evolve for some time according to Hamiltonian laws, then interrupt, destroy the correlations and proceed as before. This procedure introduces a direction of time employed in the mathematical mechanism of destroying the correlations. The mechanism is simply to ignore the correlations. Perhaps reasons could be advanced for doing so, but that is not average is different from the ensemble average; if one substitutes the ensemble average for the time average, one should make some justification for it.

It should also be mentioned that the time average is not really a sound idea, because if one calculates how long it takes for a system to go through the quasi-ergodic cycle, one finds that it is much greater (if you have a microscopic system) than the age of the Universe. Now, if we measure the pressure of a gas, usually we do not wait that long.

The entire ergodic problem, as it developed in mathematics, lost contact with physics for a very long time. The mathematical problems became of great interest in themselves, and it is not quite clear what relevance they have for physics.

(11) E. P. Wigner: private communication.

necessary for our argument here, although it might become important at another level of the theory (*)

In classical mechanics, when we have a particular Lagrangian, say a potential, we either calculate the force from it or put it into the appropriate equation and go through certain steps. In the generalized stochastic dynamics also we would have to do something similar, except that we shall have an external gradient representing the fact that every time two particles collide, or after a certain time has elapsed, all correlations are wiped out. This involves no new functions, and nothing arbitrary. And this, in a sense, is what Boltzmann did, although he did not quite say so. He was not able to say so, because he very possibly could not have believed that it is an intrinsic property of the system.

We no longer ask questions like: What is the true system? Does it really consist of particles, and does it have a definite position? (**) It is impossible to talk about a photon with a position and momentum at the same time, or to talk about a photon of a certain color and ask «Where is it?». It is just not possible. Does it mean that there is no photon? No, it merely means that we must deal with it in a somewhat different sense.

Similarly, when we deal with a thermodynamic system, it is not really true that it consists of particles, if by particles one understands all those properties which are described for billiard balls with well-defined positions and Hamiltonian evolution for the system. And that, of course, we do not have in mind. No one has ever seen the evolution of a whole collection of particles when it is in a thermal enclosure; one only sees individual particles under nonthermodynamic situations very far from equilibrium. Thus we have no experimental constraints on what this evolution should be. There is no logical reason why it must behave in a prescribed manner just because it consists of mechanical quantities.

Boltzmann could not have felt so free as to make such deductions, because in his day it would have been much too revolutionary. Not that he could not have arrived at these conclusions, but that at that time it was not very nat-

(*) We could, for example, say that the destruction of correlations, and therefore irreversibility, arise for some mysterious reason from the walls of the enclosure, but then the walls must not be a purely mechanical or Hamiltonian system, because if they were, then there would be no question of their acting in a random manner. If the walls do not obey stochastic laws, they must be Hamiltonian; then perhaps it is the air that makes things random, we do not know how. We may keep on postponing the point where the mechanism of irreversibility has to be introduced, but eventually we have to introduce something that does not obey the laws of reversible Hamiltonian mechanics.

(**) We have come to the point where we are willing to accept the notion of position or momentum for a system, and then say that there are certain systems which are as pure as one can possibly make them, in which there is no very definite value of the position. It is true that it comes from quantum mechanics, but the logic does not change.
ural to think that something beyond Hamiltonian dynamics is in fact happening to the mechanical system.

The fact that it is very difficult to obtain the actual state of the system does not obscure the fact that it has a state, if one believes that everything has a state. The total energy and momentum of the system are essentially constant, and the fact that they are constant would not change by any amount of manipulation. Boltzmann could have foreseen that, if, in his scheme, he had reversed just one collision and if $H$ had decreased in that collision, then $H$ would have increased in the opposite of that collision and it could not be true that $H$ always tends to decrease (*). One could say, of course, that the recurrence times of the collisions are infinite, hence they never reverse and so on. However, the fact is that the increase of entropy that is claimed takes place with each collision, not just after a very long period of time. Every collision between two particles increases the entropy and decreases $H$. Boltzmann was able to specify the point at which the problem must be solved by interrupting the Hamiltonian evolution. He would have foreseen that the increase of entropy (decrease of $H$) was not related to the time, unless the laws of evolution involved not only collision but collision followed by wiping out the correlations. If, however, the correlations are wiped out, it is not because the initial conditions are indefinite; it is because part of the law of evolution is such that something is destroyed.

The nonmechanical idea is the interruption of the Hamiltonian evolution of the system and the destruction of correlations. It is closely connected with the primitive ideas of the entropy, in which it was associated with disorder. Now, what is disorder? Does the fact that velocities are completely described in an unpredictable manner make the system any more disordered? There is nothing random about a situation in which each configuration is associated with every other configuration because each is represented by a point in phase space. What is really important is the distinction between a point in phase space and a distribution in phase space, and that the increase in disorder is possible only for a system which intrinsically has the possibility of some disorder.

Every configuration has some inherent scheme. If there is general disorder, that is a property of the system, and not a statement about a configuration of the system. In a given mechanical system, any configuration of the system is as good or bad as any other configuration (because nothing a priori is specified about the system except that it is mechanical), and each of them is represented by a point in phase space. Hence, the disorder consists in something more general than this; it consists in the fact that the configuration in phase space is not represented by a point, but by a distribution. Disorder is an intrinsic property attached to certain states of the system. Disorder can be seen when one is able to distinguish between two classes of states: one which is most

(*) This can be easily seen from Boltzmann's transport equation eq. (13).
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naturally ordered, such as a point in phase space; any other state has more disorder than this one (*)

Let us suppose that, in principle, we have the means of taking into account the correlations, and have sufficient information as to what happens to the system when collisions take place. Still, we shall not obtain thermodynamics from the equations of mechanics. When all the correlations are taken care of, Boltzmann's $H$-theorem will no longer be valid, because the quantity $H$ may increase (**).

As we have seen in Boltzmann's method, the increase of entropy is obtained if the correlations are destroyed, and this we must do no matter what the number of particles is so long as it is finite, without the necessity of having to take the thermodynamic limit. As long as the number of particles, harmonic oscillators, or other constituents of the system, is finite, there should arise no nonmechanical behavior (or break-down) of the system by using conventional methods. Then if the procedure is used that we have emphasized, that of interrupting the evolution after a certain time and deliberately ignoring the correlations, the entropy will be found to increase.

What is the basis for interrupting things? Why should the correlations be lost? Because the system is not entirely Hamiltonian it has stochastic elements in it. When there are just a few particles, completely isolated from their surroundings, it appears as if they behave according to the Hamiltonian law of evolution. In this, as well as in the experiments performed in the laboratory,

(*) By disorder we do not mean that complete information about the system is not available. Of course, it depends on what is meant by the objective properties of the system. If one insists that the only allowed states for the system are points in phase space, and if on the other hand it is maintained that the configuration is somewhere in between them, then we could say that there is lack of information. But if the system is of such a nature that its state is not characterized by a definite point in phase space, then it is not lack of information on our part and it is simply the nature of the system. Hence the uncertainty of the distribution characterizing the state, or the disorder, is not a case of lack of information, but rather an enriching of the kinds of states that one allows for the system. In physics, only certain classes of states have traditionally been considered as allowed, and clearly their use has been limited. If one allows wider classes of states, one can use them for more things.

(**) Some people claim that when there are large numbers of particles and certain special kinds of potentials are used, then the system is ergodic, and that one can never trace back from one configuration to another, etc. All this is somewhat unrelated to the situation. We are interested in discussing what happens in ordinary physical systems, such as the diffusion of gases, burning of carbon, melting of ice, etc., and not in considering exotic systems with peculiar special potentials. Our belief is that, irrespective of what the law of evolution is, as long as we have a reasonably large-scale sample of the system, it will behave in a reversible or irreversible manner depending upon whether it is in equilibrium or nonequilibrium; we should therefore not depend upon some special property of peculiar potentials to lead to the phenomenon which we wish to explain, because it should be seen to happen in all common, reasonably clearly understood problems.
there is the deep assumption that one can ignore the external universe. That may well be true. On the other hand, this is not a good assumption for the melting of ice in a glass of water, and we must accept the fact that the system is not sufficiently isolated from the outside, and the external universe comes into the picture. What the outside contributes is a change of temperature, thereby automatically contributing something non-Hamiltonian to the system (*)

Thus it is indeed possible to make mechanical models of systems in which the entropy increases. By mechanical, we mean models in which energy, momentum and entropy are completely defined in terms of the positions and momenta of particles. It is possible to have one unique function which determines the evolution of the system, but the evolution does not proceed according to the usual laws of mechanics. The usual laws of mechanics must be supplemented by something else. In this case one finds that the entropy can be defined at each stage as a function of positions and momenta at that time, and in general it tends to increase. It is, of course, possible that there may be certain experiments in which one might not wish to ignore the correlations between $p$'s and $q$'s; one might like to separate the system, and therefore the phase space, into several parts, in an unspecified manner. However, when any of these specifications are considered, the same thing will hold true: i.e., after collisions, some correlations would develop between the parts. We ignore these correlations, and start all over again.

One could probably define a more general $H$-theorem, not of collisions between particles but of entropies associated with the domains of phase space. One could then ask whether the entropy increases or decreases if the correlations between the domains are ignored. It is very much like the statement that if one takes an $n$-dimensional matrix, then in general there are certain eigenvalues and one can calculate $\log \rho$ or $\text{Tr} \rho \log \rho$. Suppose we decide to partition the matrix, say, into four blocks, take all the diagonal blocks, calculate each of the $\rho_i$, and then calculate $\rho_i \log \rho_i$ and sum it over $i$. It can be shown that this quantity is always larger than the $\text{Tr} \rho \log \rho$ that we calculated for the whole

(*) Boltzmann maintained that he had derived the law of change of temperature from the equations of mechanics, a conclusion with which we disagree. We are quite happy with Boltzmann's demonstration of the increase of entropy, provided it is not maintained that it has been derived from mechanics. His is a clever demonstration that $H$ decreases and the entropy increases. In fact, in some collisions $H$ increases and in others $H$ decreases, depending upon the initial conditions and the approximations that have been made for the correlations. For instance, if there are no correlations before collision, then according to the laws of mechanics, correlations might be established after collision. When these new correlations are taken into account, $H$ will not change, but if the new correlations are neglected, $H$ will decrease. If, however, there are certain correlations before collision, and they disappear after the collision and this disappearance of the correlations is neglected, then $H$ will increase. In equilibrium, of course, there is no change in correlations, and therefore in $H$. 
matrix, and any evolution of the system would lead to this result. This is exactly what happens in stochastic dynamics, which is more general than Hamiltonian dynamics (\textsuperscript{14}).

There are two essential ingredients in our prescriptions for introducing thermodynamics. One is to enrich the dynamical model of our mechanical system, and the other at a later stage is the destruction of correlations. As we have stated earlier, first we seek to enrich the mechanical system by allowing it to have impure states which are distributions in phase space (\textsuperscript{*}). In our definition of the mechanical system, the aim is to introduce those enriching elements that give us the desired properties.

The only thermodynamic property which we require that it be a model of, in our case, is the increase of entropy. From this model then, for instance, we can obtain Boltzmann's equation. This gives the logical reasons by which Boltzmann's equation is then obtained, reasons which were not available before. By this means, all special prescriptions, such as the thermodynamic limit, averaging procedures, ergodicity, etc., become superfluous.

For a system of particles, be they one or ten thousand, the thermal bath is the outside, the external universe, and the equilibrium is with the external universe. What has entropy to do with this? Entropy is something which increases under the processes we have outlined; it gives the direction of time in which the system evolves (\textsuperscript{**}). The loss or gain of information in choosing one aspect of the system over another depends on the manner of looking at it. What we have emphasized is the changed manner of looking at the Boltzmann equation. If the details can be properly modified, everything new that Boltzmann introduced was essentially correct.

8. – Prospect of a new generalized mechanics.

We have stated several times that in defining the mechanical system we wish to introduce in it those enriching elements that will give us the properties


\textsuperscript{*} It is, of course, possible that when two people perform experiments on ice, the same piece of ice may be assigned two different levels of disorder. Depending upon the conditions that are taken into account, we have two (or more) different models of the same physical system. One may want to describe a bulk or macroscopic object by two entirely different models of the system, depending upon the kind of experiments that are to be performed on it, i.e. whether one considers its mechanical properties alone or only its thermodynamic behavior. The thermodynamic behavior itself is not well defined, because one might wish to measure the chemical potential or the osmotic pressure and another might wish to measure only temperatures and pressures. Hence, two persons, depending upon their model for the system, would describe it by totally different sets of variables. If electromagnetic properties are to be looked at, still another set of variables would be necessary.

\textsuperscript{(**)} The increase of entropy is an effect of the external universe.
in which we are interested. We would like it to be a model of the increase of entropy, the essential thermodynamic property of interest to us, and from this model we obtain Boltzmann's equation. What are the most general laws that we shall tolerate for the system? When treating a many-body system in conventional Hamiltonian mechanics, for instance, we require that the Hamiltonian be a function of \( p \) and \( q \), that the particles be sufficiently far apart, so that the energy is all kinetic, and when \( q \) becomes large, \( H \) tends to the sum of individual kinetic energies. In order to simplify the problem we say that it would be nice to have only two-body forces, and when we discuss the two-particle potential there are other questions. For instance, what can it depend upon? We seek that it depend upon the relative distance only, or on the relative velocity, and be rotationally invariant, or be this or that; each of these requirements has some reason behind it, which may be altered with circumstances. The same thing applies when one considers a more general law of evolution—not just the points developing into points in phase space, but distributions developing into distributions, including points developing into distributions.

What is the most general law to consider? In what manner is this law related to mechanics? In what way can this law be specified as a function of \( p \) and \( q \), or in terms of the Hamiltonian? Undoubtedly, there is merit in considering collisions as the only entities which lead to irreversible properties like thermal conductivity, diffusion coefficient, etc. It would be nice, for instance, to be able to calculate the diffusion coefficient, given the interparticle potential rather than getting it in terms of more esoteric things. This would be attained if one takes the point of view that collision is the mechanical agency by means of which the correlations are altered, however they do not manifest themselves in thermodynamical observations, because there is no thermal conductivity or diffusion without an irreversible situation.

Where does the irreversibility come from? If the correlations are not destroyed or ignored, one could calculate three-particle and four-particle correlations (or excitations) and include the contributions from these as well. One could include still higher-order correlations, but all this does not lead to the change of entropy, to the increase of entropy (*) . Also, when it is decided to ignore or destroy correlations, it does not mean that each and every correlation must be destroyed; it may be advisable to keep some of them and ignore others. And the fact that any correlations have been ignored leads to an increase of entropy.

In the melting of ice, for instance, we are not interested in \( 10^{12} \) or more variables related to the cube of ice we are considering; our interest is primarily

(*) Taking into account higher-order correlations contributes to higher-order corrections, but it does not change the situation with respect to the entropy in the consideration of a thermodynamic or disordered system.
in the fact that ice melts, in determining what fraction of the ice melts in a
certain time, its shape at a certain time, etc. We have a system, ice, and it
melts. Can we find a dynamical model of this system in order to describe its
behavior? What can we do instead of taking 10^4 or more variables and inte-
grating them? Can we not make a theory with three or four variables?

Consider the case of black-body radiation. Whether we have a speck of
dust, a cloud of soot, a piece of stone, or a chunk of metal, all of them behave
in the same manner for the black-body radiation. Since black-body radiation
is independent of all these things, we are able to make a dynamical model for it.
In principle, we could describe the situation by considering the interaction
between the electromagnetic field and all the particles involved, however we
are not interested in this, and wish to make a dynamical model of the black-
body radiation without considering any of the other particular things. Or,
take the example of a little projectile, ejected from an apparatus, that describes
a parabola. In describing the motion of the projectile, we do not talk about all
the molecules of which the experimenter, the apparatus and the projectile are
composed.

What we wish to emphasize is that in making the dynamical model ap-
propriate to a situation related to the system, we always select the right number
of variables, and seek to describe the prescribed system with just those variables.
Of course, we make the necessary corrections or modifications for effects that
are important in a situation (be they due to gravitational attraction, evap-
oration, radiation, or a thousand things). It does not mean that another description
is not possible. When we say that this is the kind of modification that has
to be introduced to obtain thermodynamics, we mean that, with the necessary
modification of conventional mechanics, we can obtain a system in which certain
variables behave in a particular manner. In so doing we have, of course, not
lost all the other variables; what we do not require for the dynamical model
of the system, we just do not include. We alter our prescription or law in order
to assure that what is necessary for the description of the system is there, and
what is not needed can be ignored. There may not be a great change in mathe-
matical calculations, but it is the logical order that is most important.

Our basic definitions do not change essentially. The total energy is defined
in such a way that it is conserved. Similarly we define a quantity called tem-
perature, just as it has been defined since Maxwell. We also take Maxwell’s
definitions of energy and momentum, and use his or Boltzmann’s or somebody
else’s definition of entropy as a state function. Just as the relative momentum
of two particles or the sum of the squares of the linear momenta changes in the
course of time, the entropy or «disorder» also changes. We treat the entropy
as a mechanical quantity; it is defined as a distribution function of the state
of the system, and can be calculated in terms of the instantaneous quantities
or the distribution without any averaging; procedure. What is involved is
a mathematical integral which gives an average over the particular states of
the system, but it does not imply or employ any "averaging" procedures such as those that have been used, and from this integral we can obtain all the dynamical quantities such as the energy, momentum and entropy (\textsuperscript{13}).

By defining the energy as the internal energy of the system, the pressure as the pressure of the mechanical system, etc., and identifying the "disorder" of the system as its entropy, we can seek to define the entire thermodynamics of the system. By defining the free energy as another particular variable of the system and as a function of the other quantities involved, we find that the notion of temperature evolves automatically. Since it can be shown that the entropy is maximum for a certain state which is a function of the energy of the system, there occurs a parameter (the modulus of the distribution) which we call the temperature (\textsuperscript{14}). The temperature is thus defined not for just any mechanical system, but only for those mechanical systems which are in equilibrium.

One might ask whether there is a temperature if the total system is not in equilibrium, and the answer is no. There can be a subsystem with a subtemperature, but if the total system is not in equilibrium, the concept of temperature for the total system is meaningless. As for equilibrium, it means that the state of the thermodynamic system is constant in time (\textsuperscript{15}).

In this manner of looking at things, the origin of the second law of thermodynamics is within us. Why do we choose this law? Because we have seen that in natural phenomena there exists a direction of time, and we went to put it into our dynamical model (\textsuperscript{16}). When two systems interact, and if any sense

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\textsuperscript{13} See eq. (4) and the Appendix.


\textsuperscript{15} \textit{a} When the random element has reached its limit and become steady the arrow does not know which way to point. It would not be true to say that such a region is timeless; the atoms vibrate as usual like little clocks; by them we can measure speeds and duration. Time is still there and retains its ordinary properties, but it has lost its arrow; like space it extends, but does not "go on"...

\textit{b} Nothing in the statistics of an assemblage can distinguish a direction of time when entropy fails to distinguish one. [This is] the Principle of Detailed Balancing. This principle asserts that to every type of process (however minutely particularised) there is a converse process, and in thermodynamical equilibrium direct and converse processes occur with equal frequency. Thus every statistical enumeration of the processes is unaltered by reversing the time-direction, i.e. interchanging direct and converse processes. Hence, there can be no statistical criterion for a direction of time when there is thermodynamical equilibrium, i.e. when entropy is steady and ceases to indicate time's arrow (\textsuperscript{17}).

\textsuperscript{16} A. S. Eddington: \textit{The Nature of the Physical World} (Cambridge, 1929), p. 79.

\textsuperscript{17} Our aim is to make a model, or obtain a law, which would describe a natural phenomenon. Nature suggests to us the kind of law we should seek to find, rather than the law telling us what Nature is. In this case, it is Nature that is active and the Law that is passive—and it is true of all science, all understanding. The scientific law describes regularities of Nature, and must therefore have predictive power. In its predictive
is to be made of the situation, they must proceed in the same direction of time. There is only one universal time direction within any system. The correlation might develop in a certain manner at times and there may be temporal reverses, but in any explicit calculation we shall see that the direction of time is the same for both components of any interacting system, and if there are ten interacting systems it would be true of them also. Thus we have an arrow of time all over the physical universe. Since the system is no longer mechanical in the conventional sense, under the conditions we have discussed there is no question of recurrence.

In classical mechanics, the recurrence with respect to a finite number of variables comes about in a very simple manner. If the system is described by means of a certain configuration, and another configuration is obtained in the course of time, we say that a patch in phase space develops into another patch in the course of time and streams constantly; after a certain time it comes back to itself, since the phase space has only a finite volume. A patch of finite area cannot move on a constant-energy surface except by coming back to itself (*). This will no longer be true if one were to talk about the continuous expansion of the patch; something which starts out as a point, say a drop of ink in water, spreads in the course of time until a situation is obtained in which it spreads out uniformly; when this point is reached there is no further evolution of the system. The evolution ceases, or is sensibly constant at this time, and there is no question of a recurrence in which it goes back to the original situation (**). The spreading of the ink is an example of a situation in which the probability distribution spreads out; it is not a case in which a patch moves from place to place and comes back to itself. The patch may cover a different area at a different rate and a different density. The case of an ink droplet in a viscous fluid, one in which it can only spread, and the other in which it spreads and can be brought back almost to its original form, are examples of a situation in which we have the same physical components but two different physical systems. In one case, our interest is in describing only a certain class of experiments; in the other, we change the experimental situation by allowing for mo-

role, the law is the active principle and Nature assumes the passive role about which predictions are made.

In our case, the destruction of correlations is itself a part of the law that describes the situation (the increase of entropy) exactly; the destruction of correlations is not an assumption of our ignorance or incomplete observation.

(*) This, of course, presupposes that the patch in phase space develops continuously so that points which are adjacent to each other will continue to remain so for arbitrarily large future times. In other words, we assume that "mixing" will not take place.

(**) There exist, of course, experiments in which we have the situation of an ink droplet in viscous fluids which by turning slowly spreads out in a regular pattern, and on reversing the motion comes back to its original droplet form. This is an example of the situation where most of the correlations are not destroyed.
tions involving rotations, and we find that the system comes back to its original form. In the second case, therefore, it is no longer appropriate to call it a statistical system since it has more co-ordinates (*). In our formulation, therefore, there is no problem or question of the existence of mechanical reversibility; classical mechanics is reversible, while the generalized mechanics which we propose as the dynamical model of a statistical system is irreversible.

The calculation of the entropy again is quite straightforward; one simply calculates $\int f \log f \, dp \, dq$. The existence and calculation of entropy are more immediate, and it is not necessary to say anything about equilibrium. The entropy is an instantaneous function; just as one calculates energy and momentum, one may also calculate the entropy. As for the temperature, it is a characteristic parameter which occurs for a particular equilibrium state. The equilibrium state must be reached before one can find out the temperature, and a properly amended Boltzmann equation describes that situation. The expression for the entropy $\int f \log f \, dp \, dq$ must be of the form $\alpha + \beta \mu$, where $\beta = 1/T$ and $\mu$ is the chemical potential, which is also not defined until the equilibrium distribution has been attained. $\beta$ and $\mu$ are therefore the characteristic coefficients of a particular distribution of the system, and the entropy is a state function of the system.

So our attitude has consistently been that when a model is to be extended to describe a larger situation, it must acquire new characteristics. When we say that the system should be described by a new kind of expanded state, it is not due to any considerations of lack of information. Our aim is also to describe things in terms of equations of motion, time derivatives and time development, indeed in terms of a simple law. We require that the entropy, the arrow of time, be a constant over all the interacting parts of a system, because we wish to write one equation for the whole system. This is the same situation as in Newtonian physics, there being only one time for the whole system of particles, not two or many times. One can also calculate for negative times, but the law of evolution in time is not symmetrical with respect to time reversal. This is because in generalized mechanics we arrange things so that, at the end of a certain time, the correlations are destroyed. The new law can be extrapolated backwards only after we undertake a series of steps, assuring that in taking them the entropy always decreases. In this way the two directions of time are not the same, and the second law of thermodynamics essentially consists in the fact that there is an arrow of time.

(*) We have the same situation in the case of the hydrogen atom. When we consider the Balmer series, the hydrogen atom is regarded as consisting of a proton and an electron; however, when the Lamb-Rutherford shift is discussed, we consider the hydrogen atom as consisting of an infinite number of degrees of freedom. Hence, the two are not the same, system. The Schrödinger equation for the first system has nothing to do with the Schrödinger equation for the infinite degrees of freedom of the other system, even though in both cases we have hydrogen.
We should also point out that, since time is the same over the entire system, the destruction of correlations does not affect first one part of the system and then another, rather it affects all parts of the system at the same time. Hence, the entropy increases for all parts of the system in the same direction, and in the entire interacting physical universe there is one direction of time; one starts out with one time, and considers the evolution in that time. In the sense we are talking, and as we have emphasized, the direction of the increase of entropy is related to a universal entity which gives a universal arrow of time and there do not arise recurrence and reversibility in the sense of classical mechanics. Of course, there is reversibility in the elementary collision process itself, but this reversibility ceases to obtain when one includes the step that follows the collision, that is the destruction of correlations. Thus we can actually chart the increase of entropy as a function of time by considering the entropy as defined at all times for equilibrium and nonequilibrium situations.

Seen from a slightly different aspect, one might say that it is not possible to define the change of entropy uniquely, because it would depend on the particular correlations one destroys. The change of entropy always goes from zero to a maximum; depending upon the particular correlations one chooses to destroy, there will be a slow or fast rate for the change of entropy (*).

Someone might insist that the correlations which were thought to have been destroyed are still there, while another person would say that they have been destroyed. However, if we wait an arbitrarily long time, even the correlations which are in doubt will go away. In the example of the ink droplet in a viscous liquid, if we wait for a couple of years or even a couple of weeks, and then spin it back, the correlations would have been destroyed, but if we do so within a couple of hours or less, then it does make a difference as to which correlations one tended to ignore.

For the interacting universe, as we have noted, the increase of entropy is universal. The question has been asked how the arrow of time trickles down from the large scale to the small scale and vice versa. The answer is that it does not trickle down, because it goes from one subsystem to another horizon.

(*) One could ask whether there is any way of defining the change of entropy independently of the destruction of correlations. But this is still an open question. One might take a less ambitious attitude than the one we have sought to explore, by only comparing the initial and final entropies of the system. In order not to be too ambitious, it might not be necessary to talk about how the entropy increases. The entropy indeed increases, but one might eschew the discussion of the rate of increase of entropy or the continuous evolution of the system. If one is interested in talking about only the initial and the final points, one would see that it is not known how the correlations have been destroyed, although the entropy at the end is always larger than the entropy at the beginning, because of the destruction of correlations. By pursuing this argument, one does not have an arrow of time, of continuously flowing time, but arrows of time and intervals which are all in the same direction.
zontally, and permeates the entire interacting universe. If we consider the physical universe as a total system, when the correlations are destroyed the entropy of the total system increases, and, since the correlations between any two identifiable subsystems are also destroyed, clearly the entropy of the subsystem also increases. Thus the entropy is increasing everywhere in the same direction, and this is also the direction of our calculation. There is no eternal recurrence (\(^*\))!

It is not necessary, however, that a temperature be defined at all points. Of course, there exists the possibility of defining temperature when there is a continuous stream of a large number of particles. We can define a temperature field in the same way as a collection of particles approximately constitutes a field and we can talk about fluid position, fluid volume, fluid density, fluid velocity, etc. In this context, we can talk about local equilibrium which in turn defines the local temperature, rather than overall equilibrium in which the temperature cannot be defined.

In our discussion, we have assumed that the mechanical system conserves its total energy at all times. The accidental situation of its distribution may change, but the number of particles, their masses, their current, etc., remain unchanged (\(^**\)). The intrinsic structure of the system remains unchanged in the course of time, but there is no recurrence in time in the new generalized dynamics. We have chosen to make a dynamical model in which the arrow of time is intrinsic. It is part of the entire process, and there is no short or long time concerning the range of its validity. In the context we are discussing, it obtains forever, just as particles in Newtonian mechanics are eternal. Poincaré’s recurrence theorem is a purely mechanical theorem (\(^*\)). It is a very simple theorem when one understands it properly. It says that a system approaches arbitrarily close to its original configuration within a finite interval of time. A system with a finite number of degrees of freedom will tend to stage a return. If a system is spread out over a certain domain in phase space, over a certain patch on distribution, then this patch moves into another patch, the

\(^*\) Time arises from the breaking up of one experience into many; space arises by considering things at different times simultaneously; common association between time and space gives rise to causality; and from these emerge universes. (Atmānanda in Ātrāśaṃa).

\(^**\) If we consider a variable number of particles, then the dynamical number of variables would be treated differently. For instance, we shall have creation and destruction operators, and they would remain unchanged for the system. One need not create more potential fields, as there are only a certain number of fields, however one might increase or decrease the strength of the fields without changing their number, or one might alter the manner of creating and destroying kinematics, structure, etc.

\(^{12}\) H. Poincaré: Acta Mathematica, 13, 67 (1890); Le mécanisme et l’expérience, in Revue de Métaphysique et de Morale, 1, 534 (1893); see also S. Chandrasekhar: Rev. Mod. Phys., 15, 1 (1943).
patch may get deformed, or disoriented or it may move, but the area of the patch remains the same. The patch cannot cover new ground, if the total area to be covered is finite, and if it moves with a finite speed it should come back to or intersect its initial position. It may not completely superpose, but it will intersect some portion of the initial distribution in a finite amount of time. Poincaré's theorem is violated in our formulation, because the development is no longer Hamiltonian. Poincaré's theorem is another way of stating Liouville's theorem, but if the system is not Hamiltonian, Liouville's theorem also no longer applies. Similar arguments can be stated against the paradoxes pointed out by Zermelo (19) and Loschmidt (20) in relation to Boltzmann's formulation. All of these paradoxes arise because of the insistence on treating the thermodynamic systems as being subject to the laws of Hamiltonian mechanics. But if it is assumed from the beginning that the true dynamics of the system is more general, that something non-Hamiltonian must be done to give meaning to and understand the increase of entropy, then all the paradoxes and appeals to ergodic behavior become superfluous. The paradoxes arise because of the insistence that the increase of entropy is due to ignorance of elementary processes in a system of a large number of particles, although subject to Hamiltonian dynamics, when in fact one is dealing with the non-Hamiltonian dynamics of an altogether different system. Thermodynamics does not say how large or small the system should be. Both mechanics and thermodynamics are applicable to things of comparable sizes; one may have a Hamiltonian dynamics of fluids and a thermodynamics of fluids, and there would be a logical conflict if one sought to derive the latter from the former.

There is a belief that when both mechanics and thermodynamics say exactly opposite things, then thermodynamics wins. It is typified by Eddington's remark: "The law that entropy always increases—the second law of thermodynamics—holds, I think, the supreme position among the laws of Nature. If someone points out to you that your pet theory of the Universe is in disagreement with Maxwell's equations—then so much the worse for Maxwell's equations. If it is found to be contradicted by observation—well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation. This exaltation of the second law is not unreasonable. There are other laws which we have strong reason to believe in, and we feel that a hypothesis which violates them is highly improbable; but the improbability is vague and does not confront us as a paralysing array of figures, whereas the chance against a breach of the second law (i.e. against


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a decrease of the random element) can be stated in figures which are overwhelming. \textsuperscript{19}

APPENDIX

Stochastic dynamics and irreversibility \textsuperscript{20}.

The most general description of the state of a quantum-mechanical system can be specified by a density operator $\varrho$. The dynamical law for the system is formulated in terms of the density operator and may be described by a linear mapping of the set of density operators into itself. In general, this linear mapping is not necessarily a unitary transformation, however when this mapping is furnished by a unitary transformation, it represents a Hamiltonian dynamics.

A density operator satisfies the conditions

$$
\begin{align*}
(\varphi, \psi) &= (\varphi, \psi) \quad \text{Hermiticity}, \\
(\varphi, \varphi) &> 0 \quad \text{positive definiteness}, \\
\text{Tr} (\varrho) &= 1 \quad \text{normalization},
\end{align*}
$$

where $\varphi$ and $\psi$ are vectors in the Hilbert space $H$ on which the operator $\varrho$ is defined.

In order to discuss the dynamical law for $\varrho$, we consider the linear operators $\varrho$'s on $H$ as themselves forming a vector space, and we can define an inner product in this space by

$$
(\varrho_1, \varrho_2) = \text{Tr} (\varrho_1^\dagger \varrho_2).
$$

Let $L$ be the linear space of all operators $\varrho$ for which $|\varrho|^2 = \text{Tr} (\varrho^* \varrho) < \infty$. Then all density operators belong to $L$. If

$$
\varrho = a \varrho^{(1)} + (1 - a) \varrho^{(2)},
$$

where $\varrho^{(1)}$ and $\varrho^{(2)}$ are density operators and $0 \leq a \leq 1$, then by an application of Schwartz's inequality we get

$$
(\varrho, \varrho) \leq a^2 (\varrho^{(1)}, \varrho^{(1)}) + (1 - a)^2 (\varrho^{(2)}, \varrho^{(2)}) + \infty + 2a (1 - a) [(\varrho^{(1)}, \varrho^{(2)}) (\varrho^{(2)}, \varrho^{(2)})]^2 \leq a^2 + (1 - a)^2 + 2a(1 - a) = 1,
$$


where the equality holds only if \( \varphi^{(a)} = \varphi^{(a)} \) and \( (\varphi^{(a)}, \varphi^{(a)}) = 1 \). This implies that if \( \varphi \) represents a pure state, it cannot be formed as a linear combination with positive coefficients of any two distinct operators. For any \( \varphi^{(a)} \) and \( \varphi^{(b)} \) as above, \( \varphi \) is also a density operator, hence the density operators form a convex set. Let us call the set of all \( \varphi \)'s formed as above for all values of \( a \), \( 0 < a < 1 \), the line segment between \( \varphi^{(b)} \) and \( \varphi^{(a)} \). We then define the set of extremal elements of the convex set as the set of all elements which do not belong to a line segment between any two distinct elements. From this it is clear that the extremal elements of the set of all density operators is the set of operators which represent pure states, and that all other elements can be formed by positive combinations of these.

The most general dynamical transformation on the system is represented by a linear mapping of the set of density operators into itself. Since, however, there are sets of density operators spanning \( L \), this uniquely defines a linear mapping of \( L \) into itself:

\[
\varphi \rightarrow \varphi' = A\varphi.
\]

The linear mapping on \( L \) which maps the set of density operators into itself is a dynamical mapping.

The necessary and sufficient condition for a linear operator on \( L \) to give a dynamical mapping are the following:

For any set of basis vectors \( \varphi^{(a)} \) in \( H \)

\[
(A.6) \quad a) \quad (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*) = (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*)^*,
\]

\[
(A.7) \quad b) \quad \sum_r (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*) = \delta_r \delta_r',
\]

c) the operator \( \omega \) defined on \( H \) by

\[
(A.8) \quad (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*) = (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*)^*
\]

is positive definite for each choice of \( r \). In particular, this implies that

\[
(A.9) \quad (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*) > 0.
\]

When these conditions are satisfied, Hermitian operators are mapped onto Hermitian operators, the trace is preserved, and positive definite operators are mapped to positive definite operators.

Next we try to find the necessary and sufficient conditions for which the dynamical transformation represents Hamiltonian dynamics. The following conditions are equivalent.

\[ a) \] There exists a linear unitary operator \( \omega \) on \( H \) such that \( \varphi \rightarrow \varphi' = \omega \varphi \omega^* \).

That is the operator has the form

\[
(A.10) \quad (\varphi^{(a)}\varphi^{(a)}^*, A\varphi^{(a)}\varphi^{(a)}^*) = (\varphi^{(a)}\varphi^{(a)}^*, \omega \varphi^{(a)}\omega^*)^*.
\]

\[ b) \] The dynamical mapping gives a mapping of the set of pure operators into itself and induces a linear mapping on \( H \).

\[ c) \] For each member \( \varphi^{(a)} \) of any set on basis vectors in \( H \), there exists a normalized vector \( \varphi^{(a)} \) such that the dynamical transformation maps

\[
\varphi^{(a)} \rightarrow \varphi^{(a)}
\]

to \( \varphi^{(a)} \).
d) The operator $A$ of the dynamical mapping can be factored in the form

$$
(A.11) \quad \langle q^t | q^t \rangle, \quad A(p^t, \sigma^t) = (q^t, \sigma^t) \langle q^t, \sigma^t \rangle^*,
$$

where $\sigma$ and $\sigma$ are linear operators on $H$.

In addition to the above-mentioned conditions for the set of operators $A$

to give dynamical mapping, the set of operators $A$ also forms a convex set.
The set of extremal elements of this set contains those which map all pure-state operators to pure-state operators. This includes Hamiltonian mappings

as well as mappings which induce a nonlinear mapping on $H$.

So much for the general discussion of the dynamical mapping. Now we
discuss the time-dependent evolution of the system which can be represen-
ted by a continuous one-parameter semi-group of linear mappings of density
operators to density operators. In order to have a continuous time-dependent

evolution of the state of the system, we must have a family of dynamical mappings $A(t)$

$$
(A.12) \quad \rho \rightarrow \rho(t) = A(t) \rho
$$
depending on a real parameter $t$, such that

$$
(A.13) \quad A(t)sA(s) = A(t+s)
$$

for nonnegative values of $t$ and $s$, and

$$
(A.14) \quad A(0) = I.
$$

In other words, we must require that the dynamical mappings $A(t)$ form a one-

parameter semi-group. In addition we must require that the expectation value

$$
(A.15) \quad \langle q \rangle = \text{Tr} \langle q \rho(t) \rangle = \langle \sigma, A(t) \rho \rangle
$$
of the self-adjoint operator $\sigma$ belonging to $L$, for the time-dependent state $\rho(t)$,

be a continuous function of the parameter $t$. In this case the dynamics is not

reversible. In order that the dynamics be reversible, that is, if we require that
dynamical mapping of the energy have an inverse which is a dynamical mapping,

then $A(t)$ is a continuous one-parameter group of dynamical mappings $A(t)^{-1} = A(-t)$. It can be shown that when a time-dependent family of
dynamical mappings is a one-parameter group, then it is a family of Hamiltonian

mappings. On the other hand, when a family of dynamical mappings does not

form a group, it leads to a family of non-Hamiltonian mappings.

A Hamiltonian system is a reversible system, while a non-Hamiltonian

system is an irreversible system. The unitary time development of the density

matrix is characteristic of all isolated physical systems, and is a reversible

system. We are interested in a physical system $A$ which forms part of a larger

system, or interacts with another system $B$, as for instance a system of spins

interacts with the lattice in paramagnetic relaxation. In this case, it is possible
to define density matrices which refer only to the system or to degrees

do freedom of interest and thus contain just the desired information. Such a
density matrix, say \( \rho^a \), may be obtained by taking a partial trace of the density matrix \( \varrho^{ab} \) describing the complete interacting system.

The time development of \( \varrho^{ab}(t) \) is unitary, but that of \( \rho^a(t) \) is not unitary in general. The specification of \( \rho^a \) at one time \( t \), is not sufficient to determine \( \rho^a \) at any future time \( t_1 \). For this, in general, one has to refer back to the equation for \( \varrho^{ab} \), solve it to obtain \( \varrho^{ab}(t_1) \) and then evaluate \( \rho^a(t_1) \). However, there are situations of great physical interest where one writes down an equation for \( \varrho^{a} \) that gives a very close approximation to the actual time development of \( \rho^a \) and thus avoids the necessity for appealing to \( \varrho^{ab} \) at every state. One classic example of this is the Bloch equation of paramagnetic relaxation, in which the effects of the interaction of the spin \( (A) \) with the lattice \( (B) \) are lumped into a few relaxation times. The fact that the evolution of the state \( \varrho^{a} \) predicted by such an equation is nonunitary does not imply that the Hermiticity of \( \varrho^{a} \) is not preserved.

It is possible to develop a general program for relaxing systems; as an example we apply it to a system of two coupled spins. In order to obtain relaxation, we introduce a 'stirring hypothesis' with a fundamental interval \( \tau \).

Let us consider a system \( C \) composed of two subsystems \( A \) and \( B \), where \( A \) corresponds to the physical system of interest, and \( B \) corresponds to the reservoir \( s \) (or thermal bath). The internal dynamics of the system engaged in a nonequilibrium process is assumed to be described fully by a Hamiltonian, while its interaction with the surroundings is described in terms of impulsive interactions. The reservoir itself is inexhaustible, possesses a definite temperature, and is free from internal gradients (i.e., it has a uniform-temperature bath). We may write the density matrix for the complete system \( C \) as

\[
\varrho^a = \varrho^{a} \Rightarrow \varrho_{ab}^{a} \varrho_{bc}^{a} ;
\]

where the indices \( a, a' \) and \( b, b' \) correspond to the 'coordinates' of the subsystems \( A \) and \( B \), respectively.

Now consider a special class of density matrices whose dependence on \( a, b' \) is simply of the form \( \delta_{a'b'} \). Then the density matrix for the composite system is given by

\[
\varrho_{ab}^{a} = \varrho_{ab}^{b} \varrho_{bc}^{a} \delta_{b'} ;
\]

where \( \varrho^{a} \) is the density matrix for the subsystem \( A \), and \( \varrho_{bc}^{a} \delta_{b'} \) is the density matrix for the subsystem \( B \). Let us define a process of 'stirring' which associates with every general density matrix of the combined systems \( C = AB \), a special density matrix of the combined system \( C \) by the correspondence \( C \), given by

\[
\varrho_{ab}^{a} = C \{ \varrho_{ab}^{a} \} = \varrho_{ab}^{a} \delta_{b'} .
\]

For the time development of the density matrix, we start with the density matrix of the system of interest \( \varrho_{ab}^{a}(0) \) at time \( t = 0 \), extend it to \( \varrho(0)_{ab}^{a} = \varrho_{ab}^{a} \delta_{b'} \), and compute the density matrix \( \varrho^a(\tau) \) at \( \tau \) by the following unitary transformation:

\[
\varrho^a(\tau) = U^a(\tau) \varrho_{ab}^{a}(0) U^{at}(\tau) ,
\]
where

\[ U^0(\tau) = \exp \{ i\tau H^0 \} \]

and \( H^0 \) is an appropriate Hamiltonian for the combined system containing the interaction

\[ H^0 = H_A + H_S + H_{\text{int}}. \]

The quantity \( \tau \) is an appropriate parameter which is intrinsic to the system. We may now compute a new density matrix \( \rho^0(1\tau) \) for the subsystem \( A \) given by

\[ \rho_{ss'}^0(1\tau) = (U^0(\tau)\rho(0)U^0(\tau))_{ss',ss''}. \]

We extend the system \( \rho_{ss'}^0(1\tau) \) to \( \rho_{ss',ss''}^0(1\tau) \) with the help of the following relation:

\[ \rho_{ss',ss''}(1\tau) = \rho_{ss',ss''}^0(1\tau) \rho_{ss''}^0. \]

Again we compute \( U^0(\tau)\rho^0(1\tau)U^0(\tau) \), and obtain \( \rho(2\tau) \). By the same procedure we obtain a new density matrix for the subsystem of interest \( \rho_{ss'}^0(2\tau) \). We continue this process \( n \) times and obtain

\[ \rho_{ss'}^0(n\tau) = (U^0(\tau)\rho U^0(n-1\tau))U^0(\tau)_{ss',ss''}; \]

\[ \rho_{ss',ss''}(n\tau) = \rho_{ss',ss''}^0(n\tau) \rho_{ss''}^0. \]

The integer-valued variable \( n \) now serves as a \( \tau \) time parameter and as \( n \) increases the density matrix \( \rho^0(n\tau) \) of the subsystems in general, corresponds to greater and greater relaxation.

As an example, let us consider a system of two spins without an external magnetic field, when one of the spins is in contact with an infinite temperature bath. The Hamiltonian of the combined system is given by

\[ H^0 = H_A + H_S + H_{\text{int}} = \lambda(\sigma_1, \sigma_1), \quad j = 1, 2, 3. \]

Now \( H_A = H_S = 0 \), as there is no external magnetic field acting on the system; \( \lambda \) denotes the strength of coupling between the two spins.

The density matrix of the combined system at \( t = 0 \) is given by

\[ \rho^0 = \frac{1}{2} I (I + \sigma_1, \sigma_1), \]

where

\[ \rho^0 = \frac{1}{2} I + \sigma_1, \sigma_1, \]

and

\[ \rho^0 = \frac{1}{2} I. \]
where $\sigma_1$ and $\sigma_2$ are Pauli spin operators for systems 1 and 2, respectively, and $p_i, \ i = 1, 2, 3$ are the polarizations for spin system 1 in the directions 1, 2, 3.

The unitary matrix which transforms $\rho(0)$ into $\rho(\tau)$ is

$$U(\tau) = \frac{1}{2} \exp \left\{ - 3 \lambda \hbar \left[ 1 + 3 \exp \{ 4 i \lambda \} + \sigma_i, \sigma_{1 \lambda} \epsilon \exp \{ 4 i \lambda \} - 1 \right] \right\} ,$$

where $\tau$ is the fundamental interval; we have taken $\hbar = 1$. Now we can compute $\rho(\tau)$. It is given by

$$\rho(\tau) = U(\tau) \rho(0) U^\dagger(\tau) =$$

$$= \frac{1}{2} + \frac{1}{2} \left( p_{1 \lambda} \sigma_{1 \lambda} \cos^2 2 \lambda + p_{1 \lambda} \sigma_{2 \lambda} \sin^2 2 \lambda + \sin 4 \lambda P_{1 \lambda} \sigma_{1 \lambda} \sigma_{2 \lambda} \right).$$

If we now take the partial trace with respect to $\sigma_1$ we get

$$\rho^\tau(\tau) = \frac{1}{2} I + P_{1 \lambda} \sigma_{1 \lambda} \cos^2 2 \lambda.$$

By iteration, we can calculate $\rho(\nu \tau)$ which is given by

$$\rho^\tau(t) = \frac{1}{2} I + P_{1 \lambda} \sigma_{1 \lambda} \cos 2 \lambda \nu \tau,$$

where $t = \nu \tau$.

Now we may compute the stochastic matrix $A$ discussed earlier

$$\rho^\tau(t) = A \rho^\tau(0).$$

The operator $A$ is given by

$$A = \begin{pmatrix}
\frac{1}{2}(1 + a(t)) & 0 & 0 & \frac{1}{2}(1 - a(t)) \\
0 & a(t) & 0 & 0 \\
0 & 0 & a(t) & 0 \\
\frac{1}{2}(1 - a(t)) & 0 & 0 & \frac{1}{2}(1 + a(t))
\end{pmatrix},$$

where

$$a(t) = (\cos 2 \tau \lambda)^{\nu \tau}.$$

Consider the time evolution of the polarizations to be given by

$$P_{1 i}(0) \rightarrow P_{1 i}(t) = (\cos 2 \lambda \nu \tau) P_{1 i}(0),$$

$$\exp \left[ - 2t / \tau \log 2 \lambda \right] P_{1 i}(0),$$

if

$$P_{1 i}(t) = K P_{1 i}(0)$$

with

$$K = \begin{pmatrix}
a(t) & 0 & 0 \\
0 & a(t) & 0 \\
0 & 0 & a(t)
\end{pmatrix}.$$
It is easy to see that all the three polarizations $P_{11}$, $P_{12}$ and $P_{13}$ have the same relaxation time $T$ given by

$$(A.40) \quad T = \frac{1}{2 \log 2 \pi \lambda}$$

It can be seen from eq. (37) that as $t \to \infty$, all the three polarizations approach zero, which corresponds to an infinite temperature bath.

We can also see that there will not be any relaxation in the subsystem $A$ when the coupling constant $\lambda = 0$. This means relaxation does not take place unless the systems $A$ and $B$ interact with each other, and as $\lambda$ increases the rate of relaxation also increases.

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**RIASSUNTO (*)**

Si discute il problema concezionale di comprendere l’irreversibilità e la freccia del tempo. Si mette in evidenza che, generalizzando i concetti di sistema e di stato, e la meccanica che li governa, è possibile creare il contesto concezionale in cui si può capire in modo naturale l’esistenza dell’irreversibilità. La distruzione delle correlazioni è il meccanismo principale che, nell’evoluzione generalizzata data da una dinamica stocastica, porta all’aumento dell’entropia ed a tutte le conseguenze della seconda legge. Nell’Appendice si tratta il caso di due sistemi di spin interagenti e si dimostra che la distribuzione delle correlazioni e l’appropriata dinamica stocastica portano all’irreversibilità.

(*) Traduzione a cura della Redazione.

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Некоторые мысли о природе энтропии, необратимости и втором законе термодинамики.

Резюме (*). — Мы обсуждаем умозрительную проблему интерпретации необратимости и направления времени. Отмечается, что с помощью обобщения понятий системы и состояния и механики, которая управляет ими, можно создать умозрительную основу, в которой появление необратимости может быть легко понято. Нарушение корреляций представляет собой механику, который в обобщенной эволюции, определенной стохастической динамикой, приводит к увеличению энтропии и всем следствиям второго закона термодинамики. В приложении мы рассмотрели случай двух взаимодействующих однородных систем и показали, что нарушение корреляций и соответствующая стохастическая динамика приводит к необратимости.

(*) Переведено редакцией.