

Information in statistical physics *

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Abstract

We review with a tutorial scope the information theory foundations of quantum statistical physics. Only a small proportion of the variables that characterize a system at the microscopic scale can be controlled, for both practical and theoretical reasons, and a probabilistic description involving the observers is required. The criterion of maximum von Neumann entropy is then used for making reasonable inferences. It means that no spurious information is introduced besides the known data. Its outcomes can be given a direct justification based on the principle of indifference of Laplace. We introduce the concept of relevant entropy associated with some set of relevant variables; it characterizes the information that is missing at the microscopic level when only these variables are known. For equilibrium problems, the relevant variables are the conserved ones, and the Second Law is recovered as a second step of the inference process. For non-equilibrium problems, the increase of the relevant entropy expresses an irretrievable loss of information from the relevant variables towards the irrelevant ones. Two examples illustrate the flexibility of the choice of relevant variables and the multiplicity of the associated entropies: the thermodynamic entropy (satisfying the Clausius–Duhem inequality) and the Boltzmann entropy (satisfying the H -theorem). The identification of entropy with missing information is also supported by the paradox of Maxwell’s demon. Spin-echo experiments show that irreversibility itself is not an absolute concept: use of hidden information may overcome the arrow of time.

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1 Probabilities in theoretical physics

The purpose of this contribution is to present an overview of the approach to statistical mechanics based on information theory. The concept of information, intimately connected with that of probability, gives indeed insight on questions of statistical mechanics such as the meaning of irreversibility. This concept was introduced in statistical physics by Brillouin (1956) and Jaynes (1957) soon after its discovery by Shannon in 1948 (Shannon and Weaver, 1949). An immense literature has since then been published, ranging from research articles to textbooks. The variety of topics that belong to this field of science makes it impossible to give here a bibliography, and special searches are necessary for deepening the understanding of one or another aspect. For tutorial introductions, somewhat more detailed than the present one, see R. Balian (1991-92; 2004).

The meaning of probabilities, on which the concept of information relies, has long been a subject of controversy (Cox, 1946). They were introduced in the theory of games as frequencies of occurrence, directly related to the counting of configurations, and could be viewed in this framework as properties of the system *in itself*. This objective interpretation contrasts with the so-called subjective interpretation, which was initiated by Bayes and Laplace, and later on advocated by Jaynes (1957) and de Finetti (1974).

While the mathematicians who focus on the structure of the theory of probabilities do not adopt a definite position on their objective or subjective meaning, the physicists who apply them should worry about their interpretation. Most physicists have reached a spontaneous, often implicit, philosophical position inspired by their daily practice, which combines subjectivism and materialism. During the XIXth century, science was generally considered as a discovery of Laws of nature existing outside us; in such an activity the observer can be disregarded once the exploration stage is over. The development of microphysics during the XXth century has led the physicists to lay more emphasis on the role of the observer. Theory is generally regarded as the construction of a partly imperfect image of the external world in our minds, which however becomes less and less blurred, more and more faithful as science progresses. Mathematics provide the precise language which allows us to build this image; among mathematics, probabilities are the tool on which we rely to make quantitative predictions in a consistent and rational way, starting from the available information, in spite of various uncertainties. It is remarkable that the introduction of probabilities in our most fundamental theories has not prevented physics to become more and more efficient.

The existence of barriers between the reality and us, which cannot be overcome at least at the present stage of physics, has become manifest in two different theoretical frameworks. On the one hand, the unification and the simplicity of the Laws of microphysics have led to a considerable development of *statistical mechanics*. It has become clear that all properties of materials at the macroscopic scale, whether mechanical, thermal or electromagnetic, can *in principle* be explained by starting from their microscopic structure. Macroscopic theories

are then reduced to a phenomenological status. Even the Laws of thermodynamics have now lost their status of fundamental science since they can be derived from microphysics. However, describing fully a macroscopic object in terms of its microscopic constituents would require to deal with an inaccessibly large number of degrees of freedom. Neither can we control them experimentally nor even can we handle them numerically. Our only issue is a probabilistic treatment, where probabilities account for our lack of knowledge about, for instance, the positions and velocities of the molecules in a classical gas.

On the other hand, microscopic systems are governed by *quantum mechanics*. There, physical quantities are mathematically represented as recalled in section 2 by elements of a non-commutative algebra. This feature implies, in particular, Heisenberg's inequality which expresses that two non-commuting variables (such as the position and the momentum of a particle, the three components of its angular momentum, the electromagnetic field and the number of photons, or the electric and magnetic fields at the same point) necessarily display statistical fluctuations: The values of such variables cannot be specified simultaneously. Here we need probabilities not only for practical reasons as in classical statistical mechanics, but because the fundamental theory itself implies *intrinsic fluctuations*. It is not simply the *values* of the physical variables which are incompletely known, but it is the very *concept* of physical quantities which, as a matter of principle, makes them simultaneously inaccessible. Their non-commutative nature forbids us to imagine that we might fully determine them. It is impossible to assume that, underlying our probabilistic description, the state of a microscopic system at a given time could be characterized by the values of its full set of physical variables. This impossibility, which contrasts with the use of probabilities in the description of systems in classical statistical mechanics, is exemplified by Bell's inequalities and by the GHZ paradox (Greenberger et al, 1990) that we shall briefly review at the end of section 2.

In both cases, and a fortiori in quantum statistical mechanics, we are led to always treat physical quantities as random. The probabilities that govern them occur either for practical reasons because we cannot hope to describe in full detail a macroscopic system, or for theoretical reasons because quantum fluctuations prevent us from thinking that the whole set of physical quantities needed to describe a system in the quantum formalism may take well-defined values. Thus the probabilities of quantum statistical physics cannot be regarded as properties of a system as such, but they characterize the knowledge about this system of its observers in the considered conditions. The probability law adequately describing the system depends on the information available to the observer or on the number of variables that he may control. Probabilities therefore appear as having a partly subjective nature, on rather inter-subjective since two observers placed in the same conditions will assign the same probability law to a system.

Moreover, such a probabilistic description does not refer to a single object. Explicitly or implicitly we regard this object as belonging to a statistical *ensemble* of similar objects, all prepared under similar conditions and characterized by the same set of given data. This ensemble may be real, if we deal with

predictions about repeated experiments, or gedanken, if we deal with a single event.

Even though quantum mechanics requires the use of probabilities to describe systems at the microscopic scale, and even though these probabilities characterize the knowledge of observers about such systems, the theory also displays *objective features* that depend on the systems only. Indeed, as we shall recall below, the microscopic equations of motion of an isolated system are fully deterministic since the Hamiltonian operator is exactly known. (For most properties of atoms, molecules and macroscopic materials, only the very simple kinetic energy and electromagnetic interactions of the elementary constituents, the nuclei and the electrons, are relevant.) Whereas at each time the statistics of the physical quantities are accounted for by a probability law, the *evolution* of this law is governed at the microscopic scale by the reversible equation (2) below, which depends only on the object studied. The probability distribution, which characterizes our knowledge, is transferred from one time to another in a deterministic way – unless we drop information or unless part of the Hamiltonian is ill-known.

Other objective features can also emerge at the macroscopic scale. Owing to the large number of constituents, the probability distribution for many macroscopic variables can be sharply peaked. The uncertainties of the observers and the subjective aspect of probabilities can then be disregarded, and statistical predictions are replaced by objective assertions, which hold even for a single object.

The first stage of an inference consists in assigning to the system a probability distribution that accounts for the available data but is otherwise unbiased. Then, predictions are derived from this distribution by means of standard techniques of statistical physics. For instance, we may wish to predict the two-particle correlation function in a simple liquid at equilibrium, so as to understand how it scatters light; in this problem the data which characterize the macroscopic equilibrium state are the energy and particle number per unit volume. This correlation function can be deduced from the density in phase, that is, the probability distribution of the N particles of the liquid in the $6N$ -dimensional phase space. However a preliminary question should be solved: From the sole knowledge of the energy and the particle number, how should we reasonably choose this probability distribution?

2 The formalism of quantum (statistical) mechanics

We shall work within the framework of quantum statistical mechanics (Thirring, 1981, 1983; Balian, 1989), which is conceptually somewhat simpler than classical statistical mechanics. To avoid mathematical complications, we consider finite systems only and assume that the thermodynamic limit for extensive systems is taken in the end. The discreteness of spectra is then a feature which

allows to by-pass some difficulties arising in classical statistical mechanics from the continuity of the variables. For instance, the classical limit of quantum statistical mechanics generates the suitable measure in the $6N$ -dimensional phase space; this measure includes a factor $\frac{1}{N!}$ issued from the Pauli principle for indistinguishable particles, which ensures the extensivity of entropy and solves the Gibbs paradox. These facts can be explained in the framework of classical statistical mechanics (van Kampen, 1984), but less automatically. Obtaining the Third Law of thermodynamics as a consequence of statistical mechanics also requires quantization, since the behaviour at low temperatures of the entropy of a macroscopic system is governed by the low energy behaviour of its level density.

The mathematical description of a physical system in quantum mechanics involves a Hilbert space, and the physical quantities are represented by the Hermitean operators \hat{A} in this space. As indicated in the introduction, these operators, termed *observables*, play the rôle of random variables but constitute a non-commutative algebra. For instance, the three components of the spin $\frac{1}{2}$ of a fermion are described in a 2-dimensional Hilbert space by the Pauli operators $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$, which are characterized by the algebra $\hat{\sigma}_i \hat{\sigma}_j = i \sum_k \varepsilon_{ijk} \hat{\sigma}_k$; for a particle on a line, the algebra is generated by the position and momentum operators \hat{x} and \hat{p} in the Hilbert space of wavefunctions, with $[\hat{x}, \hat{p}] = i\hbar$. The specific features of quantum physics, compared to the standard probability theory or to the classical statistical mechanics, lie in this non-commutation of the observables.

In quantum mechanics, the “state of a system”, whatever formalism is used to characterize it (wavefunction, state vector, density matrix, etc), is an irreducibly probabilistic concept. As stressed in the introduction, one cannot imagine the existence of an underlying, purely objective description in terms of the values of all the physical quantities attached to the system. We are led to adhere to the Bayesian or Laplacian subjective conception of probabilities, and to regard the “state” as the best possible description of the system, which allows us to make any possible probabilistic prediction about it – or rather about the statistical ensemble to which it belongs.

A set of probabilities is equivalent to the collection of expectation values that they allow us to evaluate. A *quantum state* is thus characterized by the *correspondence* $\hat{A} \mapsto \langle \hat{A} \rangle \equiv A$ which associates with *any observable* \hat{A} its *expectation value* A in the considered situation. This correspondence has a few natural properties. The hermiticity of \hat{A} entails that A is real (quantum mechanics involves complex numbers, but physical predictions yield real numbers). For the unit operator, $\langle \hat{I} \rangle = 1$. The correspondence is linear; in fact, the linearity $\langle \hat{A} + \hat{B} \rangle = \langle \hat{A} \rangle + \langle \hat{B} \rangle$ for any pair of *commuting* observables \hat{A} and \hat{B} is sufficient to imply linearity for the whole set of observables (provided the dimension of the Hilbert space is larger than 2: Gleason’s theorem). Finally the statistical fluctuation of a physical quantity is expressed as $\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$

in terms of the expectation values (1). Imposing that $\langle \hat{A}^2 \rangle$ is non-negative for any Hermitean \hat{A} expresses that a variance cannot be negative.

For finite systems these properties are implemented through the existence of a *density operator* \hat{D} in Hilbert space which represents the state. The above correspondence from observables to their expectation values is expressed as

$$\hat{A} \mapsto \langle \hat{A} \rangle \equiv A = \text{Tr } \hat{A} \hat{D} , \quad (1)$$

where \hat{D} is a Hermitean positive operator with unit trace. The density operator thus gathers our whole probabilistic information about the full set of observables of the system. It plays with respect to observables the same rôle as a usual probability distribution does with respect to random variables. A wavefunction or a state vector $|\Psi\rangle$ appears as nothing but a special case of density operator; in this case $\hat{D} = |\Psi\rangle\langle\Psi|$ reduces to a projection on the considered pure state and the expectation values (1) read $A = \langle\Psi|\hat{A}|\Psi\rangle$. Note that, due to the irreducibly probabilistic nature of the quantum theory, there is no conceptual difference between “quantum mechanics” and “quantum statistical mechanics”, since a wavefunction is nothing but a means for evaluating probabilities.

For time-dependent problems, we need in order to make predictions to express how this information (1), given at some time, is transformed at later times. This is expressed in the Schrödinger picture by letting \hat{D} depend on time while the observables \hat{A} remain fixed. For an isolated system, with given Hamiltonian \hat{H} , the evolution of $\hat{D}(t)$ is governed by the *Liouville-von Neumann equation* of motion:

$$i\hbar \frac{d\hat{D}}{dt} = [\hat{H}, \hat{D}] . \quad (2)$$

Whereas the definition of quantum states involves both the system and the observers and has a subjective aspect because the density operator appears as a tool to make consistent predictions from the available information, the evolution refers to the system only. This purely objective nature of the evolution is made clear in the alternative Heisenberg picture, where the density operator \hat{D} remains fixed while the observables change in time according to Heisenberg’s equation of motion

$$i\hbar \frac{d\hat{A}}{dt} = [\hat{A}, \hat{H}] , \quad (3)$$

which is deterministic and reversible. Equations (2) and (3) are equivalent as regards the evolution of the expectation values (1). Heisenberg’s equation (3) exhibits better the fact that the dynamics is a property of the considered system, since it deals with the observables which represent mathematically the physical quantities belonging to this system, independently of observation. In fact, eq. (3) simply expresses that the operator *algebra remains unchanged* in time while the various observables \hat{A} evolve; this property is equivalent to the unitarity of the evolution, with the Hamiltonian as generator of the unitary motion. As another advantage, Heisenberg’s picture allows us to evaluate correlations between observables of the same system taken at different times. However, because

we focus below on information, we shall start from Schrödinger's picture rather than Heisenberg's. When expressed by means of (2) instead of (3), the evolution takes a subjective aspect, since (2) describes the transfer of information from some observables to other ones generated by a completely known dynamics. We can then modify eq. (2) so as to account for losses of information that may take place during a dynamical process.

In the *classical limit*, observables \hat{A} are replaced by commuting random variables, which are functions of the positions and momenta of the N particles. Density operators \hat{D} are replaced by probability densities D in the $6N$ -dimensional phase space, and the trace in (1) by an integration over this space. The evolution of D is governed by the Liouville equation.

To conclude this section, we show how the *irreducibly probabilistic* nature of quantum states follows from the non-commutation of the observables. Consider first two physical quantities represented by two observables \hat{A} and \hat{B} which do not commute, $[\hat{A}, \hat{B}] = 2i\hat{C}$. Since for any λ the operator $(\hat{A} + i\lambda\hat{B})(\hat{A} - i\lambda\hat{B})$ can be regarded as the square of a Hermitean operator (as obvious by diagonalization), its expectation value is non-negative, which implies $\langle \hat{A}^2 \rangle \langle \hat{B}^2 \rangle \geq \langle \hat{C} \rangle^2$. This Heisenberg's inequality sets a lower bound to statistical fluctuations (for instance, $2\hat{C} = \hbar$ for $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$ yields $\Delta\hat{x}\Delta\hat{p} \geq \hbar/2$). Accordingly, non-commuting physical quantities are *incompatible*: They cannot be measured nor even specified simultaneously.

Bell's inequalities and the GHZ paradox (Greenberger et al, 1990) also arise from non-commutation. Consider, for instance, three spins $\hat{\sigma}^{(m)}$, $m = 1, 2, 3$; define the observables $\hat{A}^{(1)} \equiv \hat{\sigma}_x^{(1)}$, $\hat{B}^{(1)} \equiv \hat{\sigma}_z^{(2)}\hat{\sigma}_z^{(3)}$, $\hat{C}^{(1)} \equiv \hat{A}^{(1)}\hat{B}^{(1)}$, and $\hat{A}^{(m)}$, $\hat{B}^{(m)}$, $\hat{C}^{(m)}$ by cyclic permutation. All of them have $+1$ and -1 as eigenvalues, the \hat{A} 's commute with one another as well as the \hat{B} 's and $\hat{A}^{(m)}$ commutes with $\hat{B}^{(m)}$. For $m \neq n$, $\hat{A}^{(m)}$ and $\hat{B}^{(n)}$ anticommute, so that the three observables $\hat{C}^{(n)}$ commute with one another. Hence, we can imagine that the 3-spin system is prepared in a pure state $|\Psi\rangle$ which is the common eigenvector of $\hat{C}^{(1)}$, $\hat{C}^{(2)}$ and $\hat{C}^{(3)}$ characterized by their eigenvalues $c^{(1)}$, $c^{(2)}$, $c^{(3)}$ all equal to $+1$. In this state, the fact that $\hat{C}^{(1)} \equiv \hat{A}^{(1)}\hat{B}^{(1)}$ takes the value $c^{(1)} = +1$ implies that $a^{(1)} = b^{(1)}$; more precisely, if we were to measure $\hat{A}^{(1)}$ and $\hat{B}^{(1)}$ simultaneously (they commute), we would find for them either the values $a^{(1)} = b^{(1)} = +1$ or the values $a^{(1)} = b^{(1)} = -1$ (with equal probabilities since the expectation value of $\hat{A}^{(1)}$ or $\hat{B}^{(1)}$ vanishes). Likewise we can assert the complete correlations $a^{(2)} = b^{(2)}$ and $a^{(3)} = b^{(3)}$. However the above definitions and algebraic relations imply the operator identities $\hat{B}^{(1)}\hat{B}^{(2)}\hat{B}^{(3)} \equiv \hat{I}$ and $\hat{C}^{(1)}\hat{C}^{(2)}\hat{C}^{(3)} \equiv -\hat{A}^{(1)}\hat{A}^{(2)}\hat{A}^{(3)}$. Hence, although the three statements $a^{(1)} = b^{(1)}$, $a^{(2)} = b^{(2)}$ and $a^{(3)} = b^{(3)}$ (in the above sense) are *separately true*, they cannot be true *together*: Since the product $\hat{A}^{(1)}\hat{A}^{(2)}\hat{A}^{(3)}$ takes the value $-c^{(1)}c^{(2)}c^{(3)} = -1$ in the considered state $|\Psi\rangle$, the simultaneous measurement of $\hat{A}^{(1)}$, $\hat{A}^{(2)}$ and $\hat{A}^{(3)}$ (which commute) is expected to yield values $a^{(1)}$, $a^{(2)}$ and $a^{(3)}$ equal to $+1$ or -1 , but necessarily with a product $a^{(1)}a^{(2)}a^{(3)} = -1$, in contradiction to the naive prediction $a^{(1)}a^{(2)}a^{(3)} = +1$

which would result from $a^{(1)} = b^{(1)}$, $a^{(2)} = b^{(2)}$, $a^{(3)} = b^{(3)}$, $b^{(1)}b^{(2)}b^{(3)} = +1$. This has been experimentally confirmed. Thus, everyday's logics is violated.

The only issue is to regard the “state” not as a property of the system alone, but as a probabilistic means for prediction. The current expression “the state of the system” that we used (and that we may still use for convenience below) is improper; it is meant as “the probability distribution (for non-commuting physical quantities) which allows us to predict the properties of the statistical ensemble in which the system is embedded”. Indeed, we can safely predict that a measurement of $\hat{A}^{(1)}$ and $\hat{B}^{(1)}$ will give $a^{(1)} = b^{(1)}$ for any element of the ensemble, and likewise for $\hat{A}^{(2)}$ and $\hat{B}^{(2)}$. However, such measurements must be performed with *different apparatuses on different samples* (described by the same state vector $|\Psi\rangle$), because $\hat{A}^{(1)}$ and $\hat{B}^{(2)}$ do not commute and hence cannot be measured nor even specified simultaneously. We cannot find in the ensemble any system for which $\hat{A}^{(1)}$ takes with certainty, say, the value $a^{(1)} = +1$ and $\hat{B}^{(2)}$ the value $b^{(2)} = +1$: The assertion that *both* $a^{(1)} = b^{(1)}$ *and* $a^{(2)} = b^{(2)}$ is meaningless. The contradiction existing between the equalities $a^{(1)} = b^{(1)}$, $a^{(2)} = b^{(2)}$, $a^{(3)} = b^{(3)}$, $b^{(1)}b^{(2)}b^{(3)} = 1$ and $a^{(1)}a^{(2)}a^{(3)} = -1$ implies that we should *not* regard the two correlations $a^{(1)} = b^{(1)}$ and $a^{(2)} = b^{(2)}$ as *intrinsic properties* of the system, but rather consider *each one as an exact prediction about a specific measurement*, namely that of $\hat{A}^{(1)}$ and $\hat{B}^{(1)}$ in one case, that of $\hat{A}^{(2)}$ and $\hat{B}^{(2)}$ in the other case, the measurements of $\hat{A}^{(1)}$ and $\hat{B}^{(2)}$ being incompatible. The state vector $|\Psi\rangle$ itself, which synthesizes all such information, does not describe intrinsic properties of the systems belonging to the considered ensemble, but rather tells us how they would behave in some experiment or another. Each assertion such as $a^{(1)} = b^{(1)}$ (which to be tested would require an interaction of a system with an apparatus measuring $\hat{A}^{(1)}$ and $\hat{B}^{(1)}$), is true *only in a given context*, which should be specified even if the measurement is not actually performed. The interpretation of quantum mechanics is thus tightly connected with measurement theory. The type of correlations that it involves cannot be accounted for in terms of hidden variables.

3 The measure of uncertainty

The knowledge embodied in a density operator \hat{D} is always probabilistic, since \hat{D} provides us only with the expectation values (1). At least some among the variances evaluated from (1) must be finite, due to non-commutation, because there exists no common eigenvector for the whole set of observables. It is therefore natural to wonder whether one density operator is more informative than another (Thirring, 1983; Balian, 1991). To this aim we associate with each \hat{D} a number, the *von Neumann entropy*

$$S_{\text{vN}}(\hat{D}) = -\text{Tr} \hat{D} \ln \hat{D}, \quad (4)$$

which measures in dimensionless units our uncertainty when \hat{D} summarizes our statistical knowledge on the system. This quantity is the quantum analogue

of Shannon’s entropy $-\sum_m p_m \ln p_m$; the latter number measures the amount of *information which is missing* on average when we wait for the reception of some message belonging to a set $\{m\}$, if each message m is expected to occur with a probability p_m (Shannon and Weaver, 1949). However, here, there will be no reception of a message since we shall never observe fully the system at the microscopic scale. The quantity $S(\hat{D})$ qualifies merely our present knowledge through \hat{D} , without reference to future observations which can change our information.

We may also interpret $S(\hat{D})$ as a measure of the *disorder* that we are facing when our information is characterized by \hat{D} . This identification of the concept of disorder with a lack of knowledge may seem questionable, since disorder seems an objective property of the system whereas information is attached to the observer. However, even in everyday’s life, we can recognize that disorder is a relative property. My desk may look quite disordered to a visitor, but it is *for me* in perfect order, if I am able to retrieve immediately any one of the many files that lie scattered on it. Likewise, a pack of cards fully mixed by a conjurer is disordered for the audience, but not for him, if he has kept knowledge of the ordering of the cards. Information theory allows us to make quantitative Maxwell’s remark about the concept of order: “Confusion, like the correlative term order, is not a property of material things in themselves, but only in relation to the mind who perceives them”.

Historically, Boltzmann was the first to identify, in many successive works, the entropy of thermodynamics with a functional of the distribution in phase space of classical statistical mechanics – even though the concept of probability was not yet fully settled. Von Neumann extended this idea to quantum physics by introducing the definition (4). The existence of these expressions inspired Shannon (1949) when he created the theory of communication, which is based on the possibility of assigning numbers to amounts of information. In this context, the subjective nature of entropy is manifest. From the fact that it measures the missing information associated with the probability distribution for the considered set of messages, it appeared that it was a general concept complementing probability. With this new interpretation as lack of information at the microscopic scale, the concept has returned to statistical physics (Brillouin, 1956; Jaynes, 1957), throwing new lights on entropy.

The von Neumann entropy is characterized by many properties which confirm its interpretation as a measure of *uncertainty*. It is *additive* for uncorrelated systems, *subadditive* for correlated ones (which means that suppressing correlations raises the uncertainty), *concave* (which means that putting together two different statistical ensembles for the same system produces a mixed ensemble which has a larger uncertainty than the average of the uncertainties of the original ensembles). The *maximum* $\ln W$ of (4) is obtained, for a finite Hilbert space with dimension W when $\hat{D} = \hat{I}/W$. Its *minimum* 0 is obtained for pure states \hat{D} , which are the least uncertain states that quantum mechanics allows, although they are still probabilistic.

4 Maximum entropy criterion

The availability of the density operator \hat{D} at a given time t_0 allows us to make any statistical prediction on the considered system (or more precisely on a statistical ensemble to which it belongs), either at the same time through (1), or at later times through (2). However, a preliminary problem arises. During the preparation of the system, before the time t_0 , only a small set of data are controlled. Let us denote as \hat{A}_i the observables that are controlled, and as A_i their expectation values for the considered set of repeated experiments. From this *partial information* we wish to *infer* other quantities. In other words, we wish to assign to the system a density operator \hat{D} , by relying on the sole knowledge of the set

$$A_i = \text{Tr } \hat{A}_i \hat{D} . \quad (5)$$

The maximum entropy criterion consists in selecting, among all the density operators subject to the *constraints* (5), the one, \hat{D}_R , which renders the *von Neumann entropy* (4) *maximum* (Jaynes, 1957). An intuitive justification is the following: for any other \hat{D} compatible with (5), we have by construction $S_{\text{vN}}(\hat{D}) < S_{\text{vN}}(\hat{D}_R)$. The choice of \hat{D}_R thus ensures that our description involves *no more information* than the minimum needed to account for the only available information (5). The difference $S(\hat{D}_R) - S(\hat{D})$ measures some extra information included in \hat{D} , but not in \hat{D}_R , and hence, not in the only known expectation values A_i . Selecting \hat{D}_R rather than any other \hat{D} which satisfies (5) is therefore the *least biased choice*, the one that allows the most reasonable predictions drawn from the known set A_i about other arbitrary quantities (1).

We may also interpret the maximum entropy criterion as the choice of the *most uncertain* state among those which satisfy the constraints (5) imposed by the data A_i , or equivalently of the *most disordered* one. This criterion may be regarded as a generalization of Laplace's *principle of insufficient reason* (or Bayes's principle), which states that equal probabilities should be assigned to all possible events in case nothing is known about the occurrence of these events. Indeed, if the Hilbert space associated with the system has a finite dimension W , the entropy is largest when \hat{D} is proportional to the unit matrix \hat{I} , so that the criterion yields $\hat{D}_R = \hat{I}/W$, describing equiprobability, in case there are no constraints (5) on expectation values.

This use of the lack of information as a tool for statistical inference has a weakness: it relies on the assumption that S_{vN} is the adequate measure of bias in statistical physics. Direct justifications of the outcome of the maximum entropy criterion, based on some requirements of consistency of the inference procedure, have therefore been given. They are discussed in detail by Uffink (1995).

An alternative direct justification relies on the introduction of a “supersystem”, made of a large number \mathcal{N} of mental copies $\alpha = 1, 2, \dots, \mathcal{N}$ of the system in hand. The statistical data are the same for all individual systems α , i.e., the observables $\hat{A}_{i,\alpha}$ ($\alpha = 1, 2, \dots, \mathcal{N}$) have the same *expectation* value A_i . This value

is identified with the value of the *average* observable $\mathcal{N}^{-1} \sum_{\alpha} \hat{A}_{i,\alpha}$ pertaining to the supersystem, which has weak statistical fluctuations (at most in $\mathcal{N}^{-1/2}$, due to non-commutation of the observables \hat{A}_i). Such an identification throws a bridge between the subjective and frequential interpretations of probabilities. The maximum entropy criterion then arises merely as a consequence of the principle of insufficient reason applied to the supersystem. This idea was introduced by Gibbs in the case where the only datum (5) is the energy: he showed that, for large \mathcal{N} , each system α is in canonical equilibrium if a microcanonical distribution is assigned to the supersystem. The extension to quantum statistical mechanics, with non-commuting observables \hat{A}_i , was worked out by Balian and Balazs (1987).

5 Generalized Gibbsian distributions and relevant entropy

For any given set of *relevant observables* \hat{A}_i , the expectation values A_i of which are known, the maximum of the von Neumann entropy (4) under the constraints (5) is readily found by introducing Lagrangian multipliers, γ_i associated with each equation (5) and Ψ associated with the normalization of \hat{D} . Its value, $S_{\text{vN}}(\hat{D}_{\text{R}})$, is reached for a density operator of the form

$$\hat{D}_{\text{R}} = \exp \left[-\Psi - \sum_i \gamma_i \hat{A}_i \right], \quad (6)$$

where the multipliers are determined by

$$\text{Tr} \hat{D}_{\text{R}} \hat{A}_i = A_i \quad , \quad \text{Tr} \hat{D}_{\text{R}} = 1 . \quad (7)$$

This least biased density operator has an exponential form, which generalizes the usual Gibbs distributions and which arises from the logarithm in the definition of the von Neumann entropy. The concavity of the von Neumann entropy ensures the unicity of \hat{D}_{R} .

The equations (7) can conveniently be written by introducing a generalized thermodynamic potential $\Psi(\gamma_i)$, defined as function of the other multipliers γ_i by

$$\Psi(\gamma_i) \equiv \ln \text{Tr} \exp \left[- \sum_i \gamma_i \hat{A}_i \right] . \quad (8)$$

The relations between the data A_i and the multipliers γ_i are then implemented as

$$\frac{\partial \Psi}{\partial \gamma_i} = -A_i . \quad (9)$$

The corresponding entropy $S_{\text{vN}}(\hat{D}_{\text{R}}) \equiv S_{\text{R}}(A_i)$ is a function of the variables

A_i (or equivalently γ_i), found from (4), (5) and (6) as

$$S_{\text{R}}(A_i) = \Psi + \sum_i \gamma_i A_i . \quad (10)$$

We term it the *relevant entropy* associated with the set \hat{A}_i of relevant observables selected in the considered situation. By construction, it measures the amount of information which is missing *when only the data A_i are available*. Eq. (10) exhibits $S_{\text{R}}(A_i)$ as the Legendre transform of $\Psi(\gamma_i)$. The relations (9) between the variables γ_i and the variables A_i can therefore be inverted as

$$\frac{\partial S_{\text{R}}}{\partial A_i} = \gamma_i . \quad (11)$$

The following examples will show that the concept of relevant entropy encompasses various types of entropies, introduced in different contexts.

6 Equilibrium thermodynamics

As stressed by Callen (1975) the Laws of thermodynamics do *not* deal with *dynamics*, but with the comparison of *the initial and the final equilibrium* states of a system. At the macroscopic level, an equilibrium state is characterized by the values A_i of a set of *extensive conservative* variables, such as energies or particle numbers. In fact, the thermodynamic laws also hold for metastable states which behave as stable states for small variations of the parameters. In such cases, the thermodynamic variables A_i include the nearly conserved quantities, which strictly speaking obey no conservation law but are conserved over the time scale of the considered process. This occurs, for instance, below a transition point for an *order parameter*, or when some a priori allowed chemical reaction does not take place under the prevailing conditions. The concept of equilibrium is thus relative: it depends on the efficiency of the interactions and many equilibria are not truly stable, but metastable over very long times. (As an extreme example, we may note that nuclear forces are effective only within each nucleus of a material; although strong, they are inhibited between one nucleus and another by the Coulomb repulsion. Nuclear equilibrium, which would imply that nuclear reactions have transformed both the light and the heavy nuclei through fusion or fission into iron nuclei, is never reached.)

Callen's statement of the *Second Law* refers to an *isolated, compound* system, in which we include the possible sources of heat or work. Each subsystem is a homogeneous piece of extensive matter. In the data A_i that characterize the initial and the final state of the whole system, the index i denotes both the subsystem and the nature of the variable (energy, number of particles of each kind, volume). Various exchanges of such quantities may take place between the subsystems under the effect of interactions. In the initial state these exchanges are prohibited by some constraints, which express that the interactions between subsystems are dropped, so that the variables A_i can be specified independently.

Later on, some interactions are restored so that some constraints are released. We wish to know the values of the variables A_i in the final equilibrium state thus reached. The answer is given by the Second Law, which postulates the existence of the *thermodynamic entropy* S_{th} , a function of the variables A_i which has the following properties (Callen, 1975). It is *additive*, being a sum of contributions of all subsystems; for each subsystem, it is *extensive* and *concave*. The final values of the variables A_i are then found by looking for the maximum of S_{th} , under constraints imposed by the initial data through the conservation laws and by possible inhibitions that forbid some exchanges between the subsystems.

This formulation of the foundations of thermodynamics is directly related to the approach to statistical mechanics of sections 4 and 5, based on information theory. It suffices to identify the thermodynamic extensive variables A_i with the expectation values (5) of the conserved observables \hat{A}_i . More precisely, the \hat{A}_i 's are the operators that commute with the Hamiltonian of the overall compound system when the interactions between the subsystems are dropped. The expectation values of the energies or of the particle numbers of the subsystems can then be frozen. The macroscopic equilibrium state, characterized by the data A_i , is identified microscopically with the most disordered state (6) accounting for these data. This surmise can be justified statistically: if no other variable than these conserved quantities A_i is controlled, reasonable predictions on any other quantity should rely on the least biased choice (6). Moreover the variances of all the macroscopic variables are then weak (of relative order N^{-1} , when N is the particle number); hence predictions about them can be made nearly with certainty, as we observe macroscopically, and they are not affected by a coarse-graining of (6). The assignment of the density operator (6) to an equilibrium state can also be justified dynamically through non-equilibrium statistical mechanics, by showing that the Hamiltonian evolution (2), while keeping the variables A_i constant, leads to the coarse-grained density operator with maximum disorder, as measured by the von Neumann entropy.

We thus identify the macroscopic *thermodynamic entropy* $S_{\text{th}}(A_i)$ with the microscopic *relevant entropy* $S_{\text{R}}(A_i)$, which was defined as the maximum of the von Neumann entropy $S_{\text{vN}}(\hat{D})$ under the constraints (5) on the thermodynamic variables A_i , frozen in the initial state. The properties of S_{th} postulated in thermodynamics are thereby found as consequences of statistical mechanics: its additivity arises from the factorization of the density operator (6) into contributions associated with each subsystem; its concavity results from the concavity of S_{vN} ; its extensivity can be proved for a wide class of interparticle interactions including the realistic interactions (Ruelle, 1969; Lieb, 1976; Thirring, 1983). The explicit form of $S_{\text{th}}(A_i)$ can also be derived from microphysics, while only its existence is asserted in thermodynamics.

When applied to the final state, the maximum entropy criterion of statistical mechanics can be worked out in two steps. In the first step S_{vN} is maximized for fixed arbitrary values of the variables A_i ; in the second step the outcome, already identified with $S_{\text{th}}(A_i)$, is maximized with respect to the variables A_i subject to constraints imposed by the conservation laws and by the possible

exchanges between subsystems. The Second Law then appears merely as the *second step* of this maximization, which leads to the largest disorder.

Eqs. (9)-(11) reduce to standard equations in thermodynamics. In particular the expression (11) of the multipliers γ_i allows us to identify them with Callen's *intensive variables* of thermodynamics; for instance, the multiplier γ associated with the energy of a subsystem is the corresponding inverse temperature. Also, Ψ is identified with a Massieu thermodynamic potential. Owing to the large number of constituents of thermodynamic system, the statistical fluctuations of the macroscopic variables are negligible, the probabilistic nature of statistical physics which underlies thermodynamics becomes invisible, so that thermodynamics appears as a deterministic theory. The thermodynamic entropy S_{th} , although it can be identified with a measure of our lack of information about the system at the microscopic scale, as well as the parameters γ entering the density operator, reach an objective status and become meaningful for a single macroscopic system.

7 Elimination of the irrelevant variables

In non-equilibrium statistical mechanics, a central problem consists in predicting the values at the time t of some set of variables A_i from the knowledge of their values at the initial time t_0 . The set of relevant observables \hat{A}_i now contains not only the constants of the motion and the quantities controlled or observed experimentally, but also other macroscopic variables, chosen in such a way that the variables A_i will eventually be coupled only to one another within a good approximation. We shall return below to the choice of this set, which for the time being we leave unspecified.

A general solution of this inference problem is provided by the *projection method* of Nakajima and Zwanzig, which we only sketch here; for a simple introduction, see Balian (1999). Since at the microscopic level the dynamics is generated by the Liouville–von Neumann equation (2), the equations of motion of $A_i(t)$ should be generated from (2) and (5). We thus need first to transform the *initial conditions* on $A_i(t_0)$ into initial conditions on $\hat{D}(t_0)$. Since at the initial time t_0 nothing else than the set $A_i(t_0)$ is specified, the least biased choice for $\hat{D}(t_0)$ is given by the maximum entropy criterion, in the form (6), (7).

From this initial state $\hat{D}(t_0) = \hat{D}_R(t_0)$, one derives the state $\hat{D}(t)$ at an arbitrary time t by solving the equation of motion (2). The relevant variables $A_i(t)$ are then found from $\hat{D}(t)$ through (5), which formally solves our inference problem. We give below a more explicit expression for this answer.

The von Neumann entropy (4) associated with $\hat{D}(t)$ remains *constant* in time, as readily checked from the unitarity of the evolution (2). This means that, if one considers *all possible observables*, *no information is lost* during the evolution. However, in general, $\hat{D}(t)$ does not keep the exponential form (6), which involves only the relevant observables \hat{A}_i . Following the procedure of sections 4 and 5, we can evaluate the lack of information associated with the

knowledge of the variables $A_i(t)$ only. It is measured by the relevant entropy (10), where the multipliers $\gamma_i(t)$ are now time-dependent and are expressed in terms of the set $A_i(t)$ through (9) or (11). By construction, we have

$$\begin{aligned} S_R[A_i(t)] &\geq S_{\text{vN}}[\hat{D}(t)] = S_{\text{vN}}[\hat{D}(t_0)] \\ &= S_{\text{vN}}[\hat{D}_R(t_0)] \equiv S_R[A_i(t_0)] . \end{aligned} \quad (12)$$

The fact that the relevant entropy is in general larger at the time t than at the initial time t_0 means that a part of our initial information on the set \hat{A}_i has leaked at the time t towards irrelevant variables. This *loss of relevant information* characterizes a dissipation in the evolution of the variables $A_i(t)$.

The construction of section 5 associates, at each time, a *reduced density operator* $\hat{D}_R(t)$ with the set of relevant variables $A_i(t)$. As regards these variables, $\hat{D}_R(t)$ is equivalent to $\hat{D}(t)$:

$$\text{Tr} \hat{D}_R(t) \hat{A}_i = \text{Tr} \hat{D}(t) \hat{A}_i = A_i(t) , \quad (13)$$

but it has the maximum entropy form (6) and thus does not retain information about the irrelevant variables. It is parameterized by the set of multipliers $\gamma_i(t)$, in one-to-one correspondence with the set of relevant variables $A_i(t)$. Regarding density operators as points in a vector space, we can visualize (fig. 1) the correspondence from $\hat{D}(t)$ to $\hat{D}_R(t)$ as a *projection* onto the manifold R of reduced states (6). (The space of states \hat{D} can be endowed with a natural metric (Balian et al, 1986) defined by $ds^2 = -d^2S = \text{Tr} d\hat{D} d \ln \hat{D}$; the correspondence $\hat{D} \rightarrow \hat{D}_R$ then appears as an orthogonal projection.) We thus consider in parallel two time-dependent descriptions of the system, the most detailed one by $\hat{D}(t)$ which accounts for all observables, and the less detailed one by $\hat{D}_R(t)$, or equivalently by the set $\gamma_i(t)$, which accounts for the variables $A_i(t)$ only, and is sufficient for our purpose.

Rather than following the motion of $\hat{D}(t)$ which involves all the complicated irrelevant variables, we wish to eliminate these variables, i.e., to follow the motion of $\hat{D}_R(t)$ on the surface R. We thus wish to project the Liouville–von Neumann trajectory of $\hat{D}(t)$ onto R. Once the operators \hat{D} are regarded as elements of the *vector space of states*, it is natural to regard the operators \hat{A} as elements of the *dual vector space, the space of observables*, the scalar product being defined by (1) and noted as

$$(\hat{A}; \hat{D}) \equiv \text{Tr} \hat{A} \hat{D} = \langle \hat{A} \rangle_{\hat{D}} . \quad (14)$$

Linear transformations in either vector spaces $\{\hat{D}\}$ or $\{\hat{A}\}$ are represented by “superoperators” acting either on their right or their left side. In particular the equation of motion (2) can be rewritten as

$$\frac{d\hat{D}}{dt} = \mathcal{L} \hat{D} , \quad (15)$$

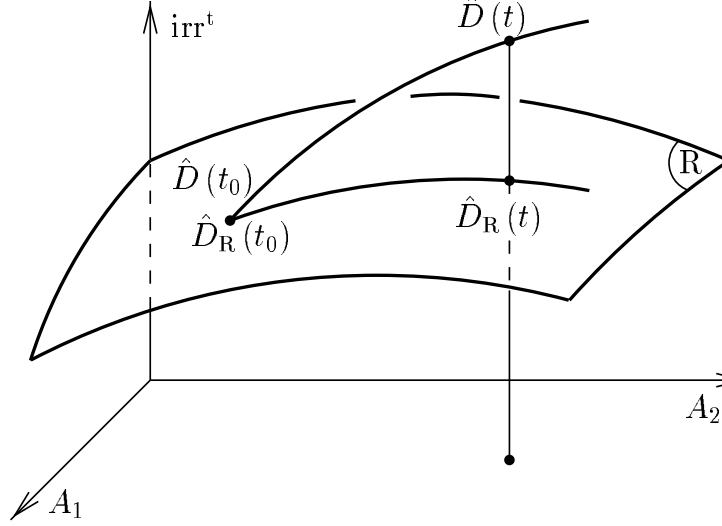


Figure 1: *The reduction of the description.* A state \hat{D} of quantum statistical physics is represented by a point in a vector space. Here the first two axes schematize the relevant variables $A_i = \text{Tr} \hat{A}_i \hat{D}$, regarded as coordinates of \hat{D} , while the third axis stands for its many irrelevant coordinates. The trajectory of $\hat{D}(t)$ is governed by the Liouville–von Neumann equation (2). The reduced state $\hat{D}_R(t)$, equivalent to $\hat{D}(t)$ as regards the relevant variables $\{A_i\}$ but maximizing the von Neumann entropy, is the intersection of the plane $A_i(t) = \text{Tr} \hat{A}_i \hat{D}$ (represented here as a line) and the surface R parameterized by the set $\{\gamma_i\}$ according to (6), (8). The trajectory of $\hat{D}_R(t)$ is obtained by projecting that of $\hat{D}(t)$ on R . It starts from the initial point $\hat{D}_R(t_0) = \hat{D}(t_0)$ and is governed by eq.(17) or its approximation (21). The von Neumann entropy is constant along the line $\hat{D}(t)$, whereas for $\hat{D}_R(t)$ information is lost towards the irrelevant degrees of freedom.

in terms of the *Liouillian superoperator* which transforms \hat{D} into $\mathcal{L}\hat{D} \equiv [\hat{H}, \hat{D}] / i\hbar$. The projection from \hat{D} to $\hat{D}_R = \mathcal{P}\hat{D}$ is implemented by means of the *projection superoperator*

$$\mathcal{P} = \hat{D}_R \otimes \hat{I} + \frac{\partial \hat{D}_R}{\partial A_i} \otimes (\hat{A}_i - A_i \hat{I}) , \quad (16)$$

where \hat{D}_R , expressed by (6), is regarded as a function of the set γ_i directly and through Ψ , and hence as a function of the set A_i through (11). A superoperator which is a tensor product $\hat{A} \otimes \hat{B}$ of operators acts on \hat{C} as $\hat{A} \text{Tr} (\hat{B} \hat{C})$ on the right side and as $\text{Tr} (\hat{C} \hat{A}) \hat{B}$ on the left side. Applied on the right side, \mathcal{P} leaves \hat{D}_R and its first-order derivatives $\partial \hat{D}_R / \partial \gamma_i$ or $\partial \hat{D}_R / \partial A_i$ invariant. Applied on the left side, it leaves the operators \hat{A}_i and \hat{I} invariant. We note the complementary

projection superoperator on the irrelevant subspace as $\mathcal{Q} = \mathcal{J} - \mathcal{P}$ where \mathcal{J} is the unit superoperator. We can then replace (15), using (16), by coupled equations for the two projected states, $\hat{D}_R = \mathcal{P}\hat{D}$, which depends on time through \hat{D} and \mathcal{P} , and $\mathcal{Q}\hat{D}$. The elimination of the irrelevant variables is then achieved, explicitly though formally, by eliminating $\mathcal{Q}\hat{D}$.

We thus find an integro-differential equation of the form

$$\frac{d\hat{D}_R}{dt} = \mathcal{P}\mathcal{L}\hat{D}_R + \int_{t_0}^t dt' \mathcal{M}(t, t') \hat{D}_R(t') , \quad (17)$$

which involves a *memory kernel*

$$\mathcal{M}(t, t') = \mathcal{P}(t) \mathcal{L} \mathcal{W}(t, t') \mathcal{L}\mathcal{P}(t') \quad (18)$$

acting in the time-dependent relevant space. This kernel depends on the *evolution superoperator* \mathcal{W} in the irrelevant space, itself defined by

$$\left[\frac{d}{dt} - \mathcal{Q}(t) \mathcal{L} \right] \mathcal{W}(t, t') = \mathcal{Q}(t) \delta(t - t') . \quad (19)$$

Eq. (17) is equivalent to the equation of motion for the relevant variables $A_i(t) = (\hat{A}_i; \hat{D}(t)) = (\hat{A}_i; \hat{D}_R(t))$, namely :

$$\frac{dA_i}{dt} = (\hat{A}_i; \mathcal{P}\mathcal{L}\hat{D}_R) + \int_{t_0}^t dt' (\hat{A}_i; \mathcal{M}(t, t') \hat{D}_R(t')) , \quad (20)$$

or for their conjugate set $\gamma_i(t)$. The first term describes the direct coupling between relevant observables. The second one, which results from their indirect coupling through the irrelevant ones, is a *retarded, memory effect* depending on the past history of the A_i 's.

We have already shown that, between the times t_0 and t , some information about the relevant variables is transferred towards the irrelevant ones, which keep memory of the initial conditions. This transfer of information is measured by (12). The *dissipation*, that is, the time-derivative of the relevant entropy, is obtained from (2), (6), (17) as

$$\frac{dS_R}{dt} = \sum_i \gamma_i(t) \int_{t_0}^t dt' (\hat{A}_i; \mathcal{M}(t, t') \hat{D}_R(t')) . \quad (21)$$

It is a *retardation effect*, associated with the history of the coupling with the irrelevant observables. (The first term of (17) does not contribute.)

Till now, we have kept the relevant observables \hat{A}_i arbitrary. Although exact, the equation (20) is in general unworkable due to retardation. If we wish to use it in practice, we should make a suitable choice of the set \hat{A}_i . Suppose this choice implies that the memory time over which $\mathcal{M}(t, t')$ is sizeable is short compared to the characteristic times of the set $A_i(t)$. This property occurs if (18) involves very many irrelevant degrees of freedom which evolve rapidly and

interfere destructively. We can then replace $\hat{D}_R(t')$ by $\hat{D}_R(t)$ and t_0 by $-\infty$ in (17). In this approximation the evolution of the relevant variables is governed by a mere differential equation at the time t

$$\frac{d\hat{D}_R}{dt} \simeq \mathcal{P}\mathcal{L}\hat{D}_R + \mathcal{K}\hat{D}_R, \quad (22)$$

where the dissipative kernel \mathcal{K} is defined by

$$\mathcal{K}(t) = \int_{-\infty}^t dt' \mathcal{M}(t, t'). \quad (23)$$

In this short-memory approximation, the dissipation (21) reduces to

$$\frac{dS_R}{dt} = \sum_i \gamma_i(\hat{A}_i; \mathcal{K}D_R). \quad (24)$$

Although $S_R(t) > S_R(t_0)$, nothing prevents (21) to be negative at some times for an arbitrary choice of the set \hat{A}_i ; at such times, relevant information (or order) which had previously been transferred to the irrelevant set and memorized there is recovered. Such a phenomenon indicates that the relevant variables have not been properly selected since they are sensitive to memory stored in the discarded variables.

However, if the short-memory approximation (22) holds, the relevant information is *irretrievably lost*: the dissipation rate (24) is positive. We understand this fact by noting that $\hat{D}_R(t)$ depends only on $\hat{D}_R(t - \Delta t)$ if the time-scale Δt characterizing the variations of \hat{D}_R or S_R in (22) or (24) can be treated as infinitesimal, but is large compared to the memory time of $\mathcal{M}(t, t')$; the much earlier initial condition $\hat{D}_R(t_0)$ is forgotten. Taking then t as the initial time in eq. (12), we find $S_R(t) \geq S_R(t - \Delta t)$ as anticipated. This *entropy production* measures a *continuous flow of order* or of information from the relevant to the irrelevant variables, which is generated by the evolution of the system.

Altogether, if we choose the set of relevant observables \hat{A}_i in such a way that the memory time associated with the dynamics of the irrelevant variables through $\mathcal{M}(t, t')$ is much shorter than the time scales associated with the motion of the relevant variables $A_i(t)$, the latter variables evolve *autonomously*. They obey the *Markovian* equation (22), and the associated entropy (24) *increases*. The quasi-instantaneous kernel \mathcal{K} accounts for the dissipative effects induced on the variables $A_i(t)$ by the eliminated ones. An adequate choice of observables \hat{A}_i , for which equations of motion of the form (22) involving through \mathcal{K} a negligible memory time are valid within a given precision, is thus not left to us. It is *imposed by the microscopic dynamics* through the possibility of separating the time scales of $A_i(t)$ and $\mathcal{M}(t, t')$. this criterion does not depend on the observers, but only on the microscopic Hamiltonian and the considered conditions. For finite systems, eq. (22) still keeps a subjective aspect even if the short-memory approximation is justified, because it deals with probabilities or equivalently with variables $A_i(t)$ that are expectation values. However, for

large systems, when statistical fluctuations are negligible, the equations of motion for the set $A_i(t)$ reach an objective status and can describe an individual system, in the same way as the equilibrium properties in thermodynamics (end of section 6). In such a situation, the increase of relevant entropy measured by the dissipation rate (24) also becomes independent of the observers, although it is microscopically interpreted as a loss of information. It quantifies the fact that the irrelevant variables act only through the quasi-instantaneous kernel \mathcal{K} , and that nothing is stored in them that could flow back towards the relevant set within any reasonable delay.

Many semi-phenomenological approaches can be recovered from microphysics through the above elimination of a set of irrelevant variables that produce no memory effects on the relevant ones. We discuss two examples in sections 8 and 9.

8 Thermodynamics of irreversible processes

Section 6 was devoted to what is usually referred to as “thermodynamics”, but should rather be called “*thermostatics*” since its Laws apply to the comparison of initial and the final state, not to the process itself which leads from one to the other. *Thermodynamics* proper provides the general laws that govern the time-dependence of the macroscopic variables, in compound systems of the type described at the beginning of section 6. These laws pertain to the thermodynamic regime, which must be sufficiently slow so that the variables $A_i(t)$ that characterize the macroscopic state at each time are the same *conservative local variables* as in section 6. However, the subsystems may now be volume elements, treated as infinitesimal but sufficiently large so that each one remains nearly at equilibrium at any time. Thus the variables A_i include the energies of the subsystems (or the energy density $\rho_E(\mathbf{r})$ in each volume element) for thermal processes; they include the numbers of constitutive particles (or their local density $\rho_N(\mathbf{r})$) for diffusive or chemical processes. They also include the density of momentum $\rho_{\mathbf{P}}(\mathbf{r})$ in hydrodynamics.

The equations of motion of thermodynamics couple the time-derivatives of the conservative variables A_i to their fluxes, which in turn are related to the gradients of the intensive variables (defined as in the end of section 6). They describe phenomena such as *relaxation* or *transport*, in physics, mechanics or chemistry. The time-scales associated with this set of macroscopic equations are large compared to the time-scales over which the subsystems reach equilibrium. Indeed, owing to their conservative nature, the variables A_i can change only if a transfer occurs from one subsystem to another, and the couplings which govern such transfers are weak compared to the interactions within each subsystem which ensure local equilibrium.

Hence, in the thermodynamic regime, the relevant variables of microscopic statistical physics should be identified with the above thermodynamic variables A_i . In the projected equations (20) that they obey, there is a clear separation of time scales and the short-memory approximation (22), (23) is valid. The

resulting coupled instantaneous equations for the set A_i can then be identified with the phenomenological equations of thermodynamics.

Since the relevant observables \hat{A}_i are the same as in section 6, their associated relevant entropy $S_R(A_i)$ is again identified with the thermodynamic entropy $S_{\text{th}}(A_i)$; its partial derivatives are related to the local intensive variables such as the local temperature, chemical potential or hydrodynamic velocity. Its rate of change, given by statistical physics as (24), is positive. This property is identified with the macroscopic *Clausius–Duhem inequality* $dS_{\text{th}}/dt \geq 0$, which can therefore be interpreted microscopically as the fact that some amount of information, or some order attached to the conservative variables is continuously lost during a dissipative thermodynamic process towards the non-conservative variables.

9 Boltzmann gas

The first historic appearance of statistical mechanics was the kinetic theory of dilute gases. In Boltzmann’s approach, the state of the gas is represented at each time by the density of particles $f(\mathbf{r}, \mathbf{p}, t)$ in the 6-dimensional single-particle phase space. Its evolution is governed by the semi phenomenological *Boltzmann equation*

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f = \mathcal{J}(f) , \quad (25)$$

the right side of which is the collision integral. It is local in space and time.

Boltzmann’s description should be regarded as macroscopic. Indeed, in order to describe at the microscopic scale a dilute gas, we should use the classical limit of quantum statistical mechanics. We indicated in section 2 that the probabilistic state is then represented by the density D in the $6N$ -dimensional phase space, which encompasses not only $f(\mathbf{r}, \mathbf{p})$ but also the 2-particle, ..., N -particle correlation functions in the single-particle phase space. Their evolution is governed by the equations of the BBGKY hierarchy, which are equivalent to the Liouville equation (the classical limit of (2)) and which, in contrast to Boltzmann’s equation (25), are invariant under time-reversal. Let us identify $f(\mathbf{r}, \mathbf{p}, t)$ with our relevant set of variables A_i , the index i standing here for a point \mathbf{r}, \mathbf{p} in phase space. Following the procedure of section 7, we can eliminate formally all the irrelevant variables, that is, all the correlations between particles. The BBGKY hierarchy then gives rise to an integro-differential equation of the type (20) for $f(\mathbf{r}, \mathbf{p}, t)$. However, in a dilute gas, the memory time entering the kernel \mathcal{W} , which describes the variations in time of the correlations, is the *duration of a collision*, since correlations are created by two-particle collisions. This duration is much shorter than the *time between two successive collisions* of a particle, which governs the evolution of $f(\mathbf{r}, \mathbf{p}, t)$. Likewise, the size of the particles is much smaller than the mean free path. The short-memory approximation is justified by this neat separation of scales. It leads on the macroscopic time-scale to an instantaneous and local equation for $f(\mathbf{r}, \mathbf{p}, t)$ of the type (22), which is identified with the Boltzmann equation (25).

The relevant entropy S_B associated with the reduced Boltzmann description, in terms of the single-particle density $f(\mathbf{r}, \mathbf{p}, t)$, is readily found by noting that D_R factorizes as a product of identical contributions from each particle and that the classical limit of a trace is an integral over phase space. We then get at each time

$$S_B \equiv S_R(f) = h^{-3} \int d^3\mathbf{r} d^3\mathbf{p} f(\mathbf{r}, \mathbf{p}) [1 - \ln h^3 f(\mathbf{r}, \mathbf{p})] . \quad (26)$$

We recognize that this *single-particle entropy* is directly related to Boltzmann's H -functional, $H \equiv \int f \ln f$, within a sign and within additive and multiplicative constants. Thus, *Boltzmann's H-theorem*, which expresses that H does not increase when f evolves according to Boltzmann's equation (25), is now interpreted as a continuous transfer of information from the single-particle data $f(\mathbf{r}, \mathbf{p})$ to correlations which are built up by each collision. In this process, $S(D)$ remains constant, expressing that no information would have been lost if we had been able to deal with the full BBGKY hierarchy, including correlations between a very large number of particles.

Boltzmann's reduced description in terms of $f(\mathbf{r}, \mathbf{p})$ is more detailed than the hydrodynamic or thermodynamic description of the gas in terms of the densities $\rho_N(\mathbf{r})$, $\rho_{\mathbf{p}}(\mathbf{r})$, $\rho_E(\mathbf{r})$ of the conserved quantities (particle number, momentum, energy). It depends at each time on one function f of six variables rather than on five functions ρ of three variables, which are obtained from $f(\mathbf{r}, \mathbf{p})$ by integration over \mathbf{p} with weights 1, \mathbf{p} and $p^2/2m$, respectively. Boltzmann's description thus remains valid in circumstances where the hydrodynamic description fails, such as shock waves and boundary layers where space variations are so rapid that local equilibrium does not exist, or very dilute gases in ballistic regimes where collisions are too rare to ensure thermalization.

Accordingly, *Boltzmann's entropy* S_B defined by (26) should not be confused with the *thermodynamic entropy* S_{th} , which for a gas is a function of the ρ 's given by the Sackur–Tetrode formula. Nor should the H -theorem for S_B be confused with the *Second Law* or with the *Clausius–Duhem inequality* for S_{th} . The latter is valid in the local equilibrium regime only (but for any material, in contrast to the H -theorem). For dilute gases in the ballistic regime, only S_B is relevant, S_{th} is useless.

Since Boltzmann's description is less reduced than the hydrodynamic one, S_B is in general smaller than S_{th} . Actually, maximization of (26) under local constraints on ρ_N , $\rho_{\mathbf{p}}$ and ρ_E provides for $f(\mathbf{r}, \mathbf{p})$ a Maxwellian form, i.e., $\ln f(\mathbf{r}, \mathbf{p})$ is a linear function of \mathbf{p} and $p^2/2m$ describing local equilibrium. When a gas is enclosed in a vessel, its irreversible evolution, which is governed by (25), leads it in a first stage to a state close to local equilibrium; Boltzmann's entropy S_B increases and eventually reaches S_{th} . Information is thus lost, not only towards the *correlations* which are not observed, but also through the evolution of $f(\mathbf{r}, \mathbf{p})$ towards a maximum entropy *Maxwellian* form. In the second stage, after the local equilibrium regime is reached, the collision term in (25) is dominated by the small deviation of $f(\mathbf{r}, \mathbf{p})$ from this form. The Chapman–Enskog method, based on the elimination of this deviation (which is formally similar to the elimination of $Q\dot{D}_R$ that leads to (17) then to (22)),

then provides the thermodynamic equations for the gas (Fourier and Navier–Stokes equations) as consequences of the Boltzmann equation. In this regime the two descriptions become equivalent; S_B and S_{th} , which remain nearly equal, both increase towards the global equilibrium entropy. The information which is being lost during this second process is the one associated with *non-uniformity* in space of the densities ρ .

10 Irreversibility and the multiplicity of entropies

The discussion of section 7 and the two examples of sections 8 and 9 elucidate the *paradox of irreversibility*, stated at the end of the XIXth century by Loschmidt, Zermelo and Poincaré: How can the reversible Liouville–von Neumann equations of motion, which underlie the behaviour of any system, give rise to the irreversible evolutions that we observe at our scale? The answer is based on information theory. Macroscopic objects are so complex at the microscopic scale that we can control or observe only an extremely tiny proportion of the entire set of variables. These experimental variables are part of a set A_i , the set of relevant variables, that we may theoretically handle (the thermodynamic densities ρ in section 8, the single-particle density f in section 9). Irreversibility is then associated with an *irretrievable leak of information (or of order)* from the set A_i towards the irrelevant variables, extremely numerous and completely out of reach. The time-derivative of the relevant entropy $S_R(A_i)$ measures this rate of dissipation.

The fact that order which is lost for us within the irrelevant degrees of freedom never returns to the relevant set is a consequence of the occurrence of *two time scales in the microscopic dynamics*. The short memory-time of the kernel \mathcal{M} in (20) is associated with the very large number of irrelevant variables and with the destructive interference of their evolutions. The longer time-scale which characterizes the motion of the relevant set A_i , including the experimentally accessible variables, is associated with some specificities of the dynamics: local conservation laws for the thermodynamic regime, large ratio between the interparticle distance and the range of forces for gases in the ballistic regime. This separation of time scales provides, within a good approximation, instantaneous equations (22) for the relevant set which, in contrast to the microscopic equations, are non-linear and irreversible. It should be stressed that the short memory in the exact equation (20) is sufficient to ensure dissipation, and that the huge number of irrelevant variables also implies that the Poincaré recurrence time is large beyond any imagination. Moreover, we have seen that, although the underlying concepts of probability, expectation value and information have a subjective nature, the resulting properties for the variables $A_i(t)$ and for the relevant entropy $S_R(t)$ become objective, depending only on the system in hand when this system is macroscopic.

Irreversibility, when analyzed at the microscopic scale, is a *statistical phe-*

nomenon. We have seen that probabilities underlie the very idea of information, a loss of which is identified with dissipation. An individual trajectory in classical mechanics, a time-dependent pure state in quantum mechanics, cannot display irreversibility, since they encompass all the degrees of freedom. Boltzmann already recognized this fact in kinetic theory, when he stressed the idea that, even when one considers a single trajectory in the $6N$ -dimensional phase space, its initial point should be regarded as a *typical* configuration belonging to some *ensemble* of macroscopically similar configurations. The logarithm of the number of these configurations is the initial entropy. The final point of the trajectory is likewise a typical configuration of a much larger set, all elements of which describe equilibrium configurations. The larger size of this set provides a quantitative interpretation of the entropy increase.

Regarding the relevant entropy as missing information has led us to assign to a given process several entropies, associated with different levels of description. For a gas we have thus characterized in section 9 the coarseness of the most detailed description, of the Boltzmann description and of the thermodynamic description by the von Neumann entropy, the Boltzmann entropy and the thermodynamic entropy, respectively. In order to understand better the mechanism which gives rise to the irreversibility of the dynamics of a classical gas, we can introduce a set of *nested reduced descriptions* (Mayer and Mayer, 1977). We start from the complete description in terms of the density D in the $6N$ -dimensional phase space, which obeys the Liouville equation. The n -th reduced description is defined by dropping all information contained in the correlations of more than n particles. Boltzmann's description is the first reduced description; the second one accounts for the two-particle correlations created by the collisions, but not for the higher order correlations; and so on. At each level, there are reduced equations of motion resulting from the BBGKY set. The associated *hierarchy of relevant entropies* $S_1 \equiv S_B, S_2, \dots, S_n, \dots, S_N \equiv S(D)$ satisfy the inequalities

$$S_{\text{eq}} \geq S_{\text{th}} \geq S_1 \geq S_2 \geq \dots \geq S_n \geq \dots \geq S(D) , \quad (27)$$

which express an increasing content of information. Their time-dependence, qualitatively shown in fig. 2, reflects the *cascade* through which correlations of more and more particles are created by successive collisions. Since two particles that have already undergone a collision have little chance to collide again for large N , due to the fact that the mean free path is much longer than the interparticle distance, information flows out from $f(\mathbf{r}, \mathbf{p})$ first to 2-particle correlations, then from 2-particle to 3-particle correlations, and so on.

Figure 2 also exhibits a non-uniform convergence. If N is fixed, S_n tends to the constant $S(D)$ at any time when n increases so as to reach N . However, under physical conditions, we have always $N \gg n$, even if we let $n \gg 1$. In this case, S_n tends for any fixed n and for long times to the equilibrium entropy S_{eq} . Thus, the amount of order $S_{\text{eq}} - S(D)$ which is in excess in the initial non-equilibrium state is eventually dissipated within the *correlations of an infinite number of particles*. This property is consistent with the way $D(t)$ converges for large t towards the equilibrium state D_{eq} of a perfect gas. Actually, for finite

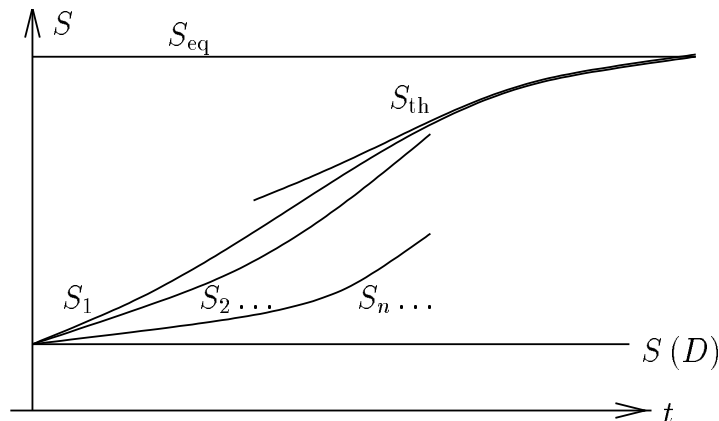


Figure 2: *Hierarchy of entropies in a gas.* Larger and larger entropies are associated with less and less detailed descriptions. The entropy $S(D)$ of the complete description remains constant for an isolated system. If the initial state is uncorrelated, Boltzmann's entropy S_1 increases (H -theorem) from $S(D)$ to the equilibrium thermostatic entropy S_{eq} , evaluated for the initial values of the energy, particle number and density of the gas. It is smaller than the thermodynamic entropy S_{th} , a function of the local densities of energy, particles and momentum, but both remain nearly equal after the distribution $f(\mathbf{r}, \mathbf{p}, t)$ has become Maxwellian (local equilibrium regime). The entropies $S_2, S_3 \dots S_n$ accounting for 2-, 3-, \dots n -particle correlations evolve like S_1 ; they are at each time smaller and smaller with n and increase later and later.

$N, D(t)$ cannot reach D_{eq} since their entropies differ. However, if N is made large first, $D(t)$ becomes equivalent for large t to D_{eq} as regards $f(\mathbf{r}, \mathbf{p})$ (a Maxwellian distribution) and as regards all the correlations of a *finite* number n of particles (these correlations are negligible).

Note that the entropies of the above hierarchy are purely theoretical objects. The only ones that experiments may reach, more or less indirectly, are $S_{\text{B}}, S_{\text{th}}$ and S_{eq} , depending on the circumstances.

11 Spin echoes

Let us return to the paradox of irreversibility. Consider a gas, enclosed in a vessel and prepared at the initial time $t_0 = 0$ in an off-equilibrium state (for instance with a non-uniform density). At the time τ , it has reached equilibrium. If we were able to reverse suddenly the velocities of all the particles, we would recover the initial state at the time 2τ . Such a violation of the arrow of time in thermodynamics cannot be experimentally achieved, because the needed inversion of the individual velocities is not feasible. Anyhow, since the number of microscopic configurations associated with the initial non-equilibrium state is enormously smaller than the number of those associated with the final equi-

librium state, the above hypothetical reversal of velocities should be performed rigorously, which is unthinkable; a small deviation would lead at the final time 2τ to a configuration having equilibrium features at the macroscopic scale, in contrast to the initial off-equilibrium configuration.

Nevertheless, similar paradoxical evolutions which violate at a macroscopic scale the laws of thermodynamics have been built up, through subtle experiments of nuclear magnetism (Abragam and Goldman, 1982). The nuclear spins $\hat{\mathbf{s}}_i$ ($i = 1, 2, \dots, N$), the value s of which is a half-integer, lie in an external magnetic field permanently applied along the z -axis. They undergo a Larmor precession around this axis with angular frequency ω_0 along z and proportional to the field. The only quantities that can be observed in practice are the components of the total magnetic moment $\mathbf{M}(t)$, equal in dimensionless units to the expectation value over the density operator $\hat{D}(t)$ of the total spin

$$\hat{\mathbf{M}} \equiv \sum_i \hat{\mathbf{s}}_i . \quad (28)$$

One can act on the system only by means of time-dependent external fields coupled to $\hat{\mathbf{M}}$. One thus handles simultaneously all the spins, which globally rotate. In particular, application at time t of a brief magnetic pulse along some axis during a controlled delay allows one to suddenly perform any overall rotation, with a given angle Ω around a given direction $\mathbf{\Omega}/\Omega$. This pulse modifies the density operator $\hat{D}(t)$ into $\hat{U}D(t)\hat{U}^\dagger$, where $\hat{U} = \exp(i\mathbf{\Omega} \cdot \hat{\mathbf{M}})$ is the unitary transformation describing the considered rotation.

The Hamiltonian has the following form

$$\hat{H} = \hbar\omega_0 \hat{M}_z + \sum_i \hbar\delta\omega_i \cdot \hat{\mathbf{s}}_i + \hat{V}_{ss} + \hat{V}_{sl} . \quad (29)$$

Its first term generates the *Larmor precession* $d\mathbf{M}/dt = \boldsymbol{\omega}_0 \times \mathbf{M}$ around z . The next terms are responsible for three different mechanisms of relaxation of \mathbf{M} .

(i) The applied field is *not quite uniform*. Each spin $\langle \hat{\mathbf{s}}_i \rangle$, depending on its location, undergoes a Larmor precession with angular frequency $\omega_0 + \delta\omega_i$. If all the spins $\langle \hat{\mathbf{s}}_i \rangle$ lie initially along the x -axis, they precess at different speeds, nearly in the xy -plane, and thus get gradually out of phase. Hence their sum $\mathbf{M}(t)$ spirals down to zero in the vicinity of the xy -plane. If we denote as δ the statistical fluctuation of $\delta\omega_{iz}$ (the average over i of which vanishes) the relaxation time for this process is $1/\delta$.

(ii) The *spin-spin* contribution \hat{V}_{ss} to (29) is the sum of the two-body dipolar interactions. Under the experimental conditions where ω_0 is sufficiently large, the part of \hat{V}_{ss} which does not commute with \hat{M}_z is ineffective. These pairwise interactions play for the spins the same role as the interparticle interactions for a gas. A “flip-flop” process, which changes the configuration $\uparrow\downarrow$ of a pair into $\downarrow\uparrow$, is the equivalent of a collision, which changes the momenta of two particles in a gas. This mechanism gradually creates correlations between two, then three spins, and so on. By a process similar to the one described at the end of section 10, the state of the N -spin system thus tends to a maximum entropy

Boltzmann–Gibbs distribution $\hat{D}_{\text{eq}} \propto \exp(-\beta\hat{H})$, apart from invisible many-spin correlations. The spin temperature $1/\beta$ depends only on the initial energy of the spins. The relaxation time for this process is traditionally denoted as T_2 .

(iii) The *spin-lattice* contribution \hat{V}_{sl} to (29) couples the nuclear spins to the other degrees of freedom (the “lattice”), such as the phonons in a solid. It tends to thermalize the nuclear spins, imposing them the lattice temperature. Its associated relaxation time T_1 is much longer than the duration of the spin echo experiments, owing to the weakness of the coupling between the nuclear spins and the other variables of the material. We shall thus disregard this term.

The oldest type of spin echoes was discovered by Hahn soon after the birth of nuclear magnetic resonance. Such spin echo experiments are performed on liquids, the disorder of which smoothes out the interactions \hat{V}_{ss} . The Hamiltonian thus reduces to the first two Zeeman terms of (29). One starts from an equilibrium state, at a sufficiently low temperature so that all spins are practically oriented along z . By a pulse $\pi/2$ applied along y just before the time $t_0 = 0$, one generates an off-equilibrium pure *initial state* $\hat{D}(0)$ with magnetization $M_x(0)$ having the largest possible value Ns , and $M_y = M_z = 0$. As indicated above under (i), the magnetization $\mathbf{M}(t)$ *relaxes* under the effect of the heterogeneity of the field. After a number of turns larger than ω_0/δ , at some time τ larger than $1/\delta$ (but smaller than T_2 and T_1), all three components of \mathbf{M} have reached 0. If we imagine we have followed the motion at the microscopic scale, the state $\hat{D}(t)$ has remained pure: each one of the N vectors $\langle \hat{\mathbf{s}}_i \rangle$ has kept the maximum length s ; its component along z is negligible as δ/ω_0 , while it points out in some direction in the xy -plane. This direction is determined by the local magnetic field, i.e., by $\delta\omega_{iz}$. Nothing seems to distinguish this state from the reduced state \hat{D}_{R} which describes thermodynamic equilibrium at large temperature. While the entropy $S(\hat{D})$ has kept its initial value 0, the relevant entropy $S(\hat{D}_{\text{R}}) = S_{\text{R}}(\mathbf{M} = 0)$ associated with \mathbf{M} has reached the largest possible value $N \ln(2s + 1)$. The system seems “dead” since only $\mathbf{M} = 0$ is observed in practice.

However, superimposed to the permanent magnetic field, a pulse π along x is applied at the time τ . The components $\langle \hat{s}_{ix} \rangle$, $\langle \hat{s}_{iy} \rangle$, and $\langle \hat{s}_{iz} \rangle \simeq 0$ are quasi suddenly changed by the corresponding unitary transformation into $\langle \hat{s}_{ix} \rangle$, $-\langle \hat{s}_{iy} \rangle$, and $-\langle \hat{s}_{iz} \rangle \simeq 0$. Hence, the spins which precess faster than the average Larmor flow because $\delta\omega_{iz} > 0$, and which were therefore ahead at the time τ by some angle, are now behind at the time $\tau + 0$ by just the same angle. Likewise, the spins that precess slower have been brought forward by the pulse. Hence, after a second time lapse τ , during which the precession goes on with the same local frequency, all the spins reach the initial direction along x , and the total magnetization \mathbf{M} *returns to its largest possible value* Ns at the time 2τ . Between the times τ and 2τ , the initial order has progressively been recovered, the relevant entropy $S_{\text{R}}(\mathbf{M})$ has decreased from $N \ln(2s + 1)$ to 0. A single *macroscopic manipulation*, the application of the pulse π along x at τ , has been sufficient to produce an evolution which *violates the thermodynamic surmise*, as

would have done the unfeasible reversal of velocities for a gas. This paradoxical evolution can be understood only by keeping track of *all* the microscopic spin degrees of freedom.

In this spin echo experiment, the order about \mathbf{M} , lost between the time 0 and τ and recovered between τ and 2τ , is associated with the *correlation for each spin*, which during the motion is established between the direction of the vector $\langle \hat{\mathbf{s}}_i \rangle$ in the xy -plane and the value $\delta\omega_{iz}$ of the z -component of the local magnetic field. The very large number $\omega_0\tau/\hbar$ of revolutions of the spins that take place during the time τ produces a configuration of directions of spins $\langle \hat{\mathbf{s}}_i \rangle$ which seems to be just a sample picked up at random within the truly dead ensemble \hat{D}_R describing equilibrium. Even if we are given the full available information, to wit, the seemingly dead density operator $\hat{D}(\tau)$ issued from $\hat{D}(0)$ and the Hamiltonian \hat{H} that generated the evolution, we would have an extreme difficulty to uncover, among this huge amount of data, the crucial correlations between $\langle \hat{\mathbf{s}}_i \rangle$ and $\delta\omega_{iz}$. Our situation is the same as that of the audience of a conjuring show, who are unable to detect how the shuffling process has retained some hidden order in a pack of cards. The experimentalist has also the same pieces of information, $\hat{D}(\tau)$ and \hat{H} , but like the conjurer he acknowledges therein that the directions of the $\langle \hat{\mathbf{s}}_i \rangle$'s are not random but are correlated with the $\delta\omega_{iz}$'s. Indeed, he is aware of the initial conditions and of the history of the system which destroyed the visible order, an information which is equivalent to the knowledge of the correlations between $D(\tau)$ and \hat{H} , but easier to analyse. Relying on this knowledge, he is able to bring back the order buried in these correlations into the simple macroscopic degrees of freedom \mathbf{M} .

He succeeds in this task owing to a specificity of the motion: it is two-dimensional except during a pulse, and we can see that the rotation \hat{U} around the x -axis has an effect akin to a time reversal. Indeed, noting that the final state is invariant under the rotation $\hat{U} = \hat{U}^\dagger$ around x , we can write the evolution operator between the times 0 and 2τ as

$$\hat{U}^\dagger \exp\left(-i\hat{H}\tau/\hbar\right) \hat{U} \exp\left(-i\hat{H}\tau/\hbar\right) = \exp\left(-i\hat{U}^\dagger \hat{H} \hat{U} \tau/\hbar\right) \exp\left(-i\hat{H}\tau/\hbar\right) . \quad (30)$$

Since the components ω_{ix} of the field have little effect, we can write

$$\hat{U}^\dagger \hat{H} \hat{U} \simeq -\hat{H} . \quad (31)$$

This change of sign has the same effect as a *time-reversal* taking place during the second part of the process, which therefore brings us back to the initial states at the time 2τ .

After the time 2τ , the evolution is exactly the same as after the initial time 0 and $\mathbf{M}(t)$ returns to zero. The operation can then be *iterated*, and the measurement of the length of $\mathbf{M}(t)$ provides a sequence of peaks. Their height slowly decreases due to the other relaxation mechanisms that we have neglected on the time scale $1/\delta$. Spin echoes have thus become a current technique in nuclear magnetic resonance to determine relaxation times with precision and thus explore matter.

At the epoch of their discovery, these spin echoes were regarded as somewhat miraculous since they violated thermodynamics: They appeared as an exceptional macroscopic phenomenon that can be explained only through the microscopic dynamics. Full knowledge of $\hat{D}(\tau)$ and of \hat{H} is needed here, whereas the thermodynamic phenomena can be described in terms of the reduced state \hat{D}_{th} and of \hat{H} only. We may, however, argue that the order which is retrieved was not very deeply hidden. It lay at the time τ in the rather trivial set of correlations between the orientation of each spin and the size of the corresponding local field. It is natural to think that the relaxation induced by the *spin-spin interactions* should in actual fact be incurable, in the same way as the collision-induced relaxation in a gas. Nevertheless, quite surprisingly, spin-echo experiments of a different type have been performed, in which the “*death*” of spins ($\mathbf{M} \rightarrow 0$) caused after the relaxation time T_2 by the term \hat{V}_{ss} of (29) is followed by their “*resurrection*” (Abragam and Goldman, 1982). We only sketch here the basic ideas. The considered experiments are performed on solids, for which \hat{V}_{ss} is significant. The applied field is sufficiently uniform so that the duration of the experiment is much shorter than $1/\delta$. The Hamiltonian (29) can therefore be simplified into $\hat{H} = \hbar\omega_0\hat{M}_z + \hat{V}_{\text{ss}}$. The experiment begins as in Hahn’s spin echoes by the preparation of an initial state with $M_x = Ns$, $M_y = M_z = 0$, then during the Larmor precession by its decay, taking now place under the effect of \hat{V}_{ss} . At a time τ larger than T_2 , the magnetization is lost as above, but now the relaxation has taken place (as in the case of gases) through a cascade of flip-flop transitions involving more and more spins. The initial order has dissolved into complicated many-spin correlations, and the density operator

$$\hat{D}(\tau) = e^{-i\hat{H}\tau/\hbar}\hat{D}(0)e^{i\hat{H}\tau/\hbar} \quad (32)$$

is equivalent, as regards observables involving a finite number of spins, to a “dead” equilibrium state with large temperature.

After the time τ , a sequence of suitably chosen brief pulses and lasting time-dependent fields referred to as a “*magic sandwich*”, is applied for a duration τ' . Thus, during this period, the Hamiltonian becomes $\hat{H} + \hbar\boldsymbol{\omega}(t) \cdot \hat{\mathbf{M}}$ where $\boldsymbol{\omega}(t)$ is proportional to the time-dependent applied field. The remarkable fact is the possibility of choosing $\boldsymbol{\omega}(t)$ in such a way that the unitary operator which describes the evolution between the times τ and $\tau + \tau'$ has approximately the form

$$T \exp \left\{ -i \int_{\tau}^{\tau+\tau'} dt \left[\hat{H}/\hbar + \boldsymbol{\omega}(t) \cdot \hat{\mathbf{M}} \right] \right\} \simeq \exp \left[i\lambda\hat{H}\tau'/\hbar \right] \quad (33)$$

(T denotes time-ordering). The coefficient λ is positive, so that, as in eqs. (30) (31), the effect of the magic sandwich $\boldsymbol{\omega}(t)$ is to replace τ' by $-\lambda\tau'$, thus *changing effectively the arrow of time* in the considered interval. The actual realization of eq. (33) has needed great ingenuity, because the dipolar interactions contained in \hat{H} involve pairwise interactions whereas the external operations are represented by a mere field coupled to $\hat{\mathbf{M}}$ only.

As an example, in one of the experiments performed, $\boldsymbol{\omega}(t)$ in (33) describes a magic sandwich consisting of three successive operations: (i) at the time τ ,

a pulse $\pi/2$ along y is exerted, represented by the operator U ; (ii) between the times τ and $\tau + \tau'$, a radiofrequency field along x , with a frequency ω_0 and an intensity $\hbar\omega'$ is applied; in the Larmor rotating frame, it provides a contribution $\hbar\omega'\hat{M}_x$ to the Hamiltonian; (iii) at the time $\tau + \tau'$ a pulse $-\pi/2$ is applied along y . The evolution operator (33), written in the rotating frame, is thus

$$\hat{U}^\dagger \exp \left[-i \left(\hat{V}_{ss}/\hbar + \omega' \hat{M}_x \right) \tau' \right] \hat{U} = \exp \left(-i \hat{U}^\dagger \hat{V}_{ss} \hat{U} \tau' / \hbar - i \omega' \hat{M}_z \tau' \right) . \quad (34)$$

If ω' is sufficiently large, the part of $\hat{U}^\dagger \hat{V}_{ss} \hat{U}$ which does not commute with M_z is negligible, and one finds

$$\hat{U}^\dagger \hat{V}_{ss} \hat{U} \simeq -\frac{1}{2} \hat{V}_{ss} , \quad (35)$$

which replaces here (31). The last term in (34) amounts to a trivial Larmor rotation. Thus (33) is satisfied (in the rotating frame) with $\lambda = \frac{1}{2}$.

After the time $\tau + \tau'$ the evolution is again governed by the sole Hamiltonian \hat{H} . Hence, provided τ' is larger than τ/λ , we can introduce a delay τ'' such that $\tau - \lambda\tau' + \tau'' = 0$, for which the full evolution operator from $t = 0$ to $t = \tau + \tau' + \tau''$, found from (32) and (33) is nearly the unit operator. The magnetization $\mathbf{M}(\tau + \tau' + \tau'')$ thus returns to its initial value $\mathbf{M}(0)$ although it had previously decayed to zero during the time τ . Here again the arrow of time is challenged.

The features of this process are the same as in Hahn's echoes, in particular the *recovery of hidden order* and the need for explaining this phenomenon to rely on *all the microscopic degrees of freedom*, although the observations and the manipulations concern only the macroscopic quantities \mathbf{M} . However, here, the order that is experimentally retrieved had been transferred by the evolution towards extremely complicated correlations of large numbers of spins, and the initial decay seemed genuinely irreversible as in the case of a gas. Indeed, for nearly all experiments which can be realized in practice, the state $\hat{D}(\tau)$ which involves these special correlations keeping memory of $\hat{D}(0)$ gives the same predictions as the reduced equilibrium state \hat{D}_R . Nevertheless, the magic sandwich manipulation, which is rather tricky, transforms back these special correlations of $\hat{D}(\tau)$ into the initial order restored in $\hat{D}(\tau + \tau' + \tau'')$. The magic sandwich experiments achieve, for spins, the analogue of the hypothetical reversal of velocities for a gas; quite remarkably, it is simply the application of some special uniform time-dependent magnetic fields which overcomes here the apparent disorder generated by the interactions.

12 Conclusion

An analysis of various physical processes where we made use of the information concept has led us to stress the *relative* nature of entropy, identified with missing information. Depending on the circumstances, macroscopic phenomena

should be described in terms of different sets of relevant variables. Different associated entropies are thus introduced, even for the same system. The entropy of thermodynamics is only one of them.

Dissipation, which is also relative, is measured by the increase of some relevant entropy. It characterizes the irreversibility of a macroscopic process, and can be interpreted as an irretrievable leak of information towards inaccessible degrees of freedom. Since information, as well as probability, is a concept associated with the knowledge of observers about an object rather than with the object in itself, thermodynamic notions such as entropy and dissipation have at the microscopic level a *subjective* aspect.

This subjective character is exemplified by the spin-echo experiments, which show that *irreversibility itself is relative*. In such circumstances the loss of memory which accompanies an irreversibility may be overcome and a hidden order, which keeps track of the initial state, may come into view.

However, in less exotic circumstances, for instance, for systems displaying a collective motion or for materials that can be described by thermodynamics, it is possible to select among the huge set of microscopic variables some subset of relevant variables which obey autonomous equations of motion. The latter dynamical equations are often identified with phenomenological equations. Their establishment from microphysics involves approximations, such as the short-memory approximation, but they can hold with a high precision if there is a clear-cut separation of time-scales which allows the elimination of irrelevant variables. The existence of these variables manifests itself through quasi-instantaneous dissipative effects. Such a reduction of the description brings in new features, which differ *qualitatively* from those of microphysics, especially for macroscopic systems: continuity and extensivity of matter at our scale, irreversibility and non-linearity of the equations of motion, existence of phase transitions, enormous variety of behaviours in spite of the simplicity of the elementary constituents and in spite of the unicity of the microscopic Laws. Due to the change of scale, the statistical fluctuations of the relevant observables are small compared to experimental or computational errors. The *very nature of our description* is thus changed. Although the underlying, more fundamental description yields predictions having subjective features due to the necessary use of probabilities, it gives way to a reduced description that no longer involves the observer. Since the variances are negligible, the physical quantities do not need to be regarded as random variables. The expectation values $\langle \hat{A}_i \rangle$ which obey the reduced dynamics can be interpreted merely as values actually taken in a given system. Their equations of motion then directly apply to individual objects, without reference to a statistical ensemble. In spite of the disappearance of probabilities at the macroscopic scale, the relevant entropy survives as a quantity measurable indirectly through its variations (11) and characterizing equilibrium, as well known in thermodynamics. Its probabilistic and subjective origin, its interpretation as missing information are not apparent; neither are they for the other variables, the expectations A_i and the parameters γ_i of the microscopic probability law. Actually all these quantities had already been

introduced in thermodynamics at the macroscopic level, but the advent of statistical mechanics gave us a deeper understanding. Indeed, statistical mechanics is a major tool of reductionism; its use explains the *emergence* at a larger scale of new properties, new concepts and even different interpretations of physical statements, such as here the emergence of objectivity from a microscopic theory based on the subjective concepts of probability and information. Likewise, treating quantum measurements as a problem of statistical mechanics (Allahverdyan et al, 2003) shows how ordinary probabilities emerge from the underlying irreducible extension of probabilities which accounts for the non-commutation of quantum observables.

Let us finally recall that the identification of entropy with a lack of information or equivalently with disorder has contributed to the elucidation of the paradox of *Maxwell's demon*, which gave rise to discussions for more than one century. An important step was the recognition of the equivalence between information and negentropy (Brillouin, 1956). The entropy of a system spontaneously increases; however it may be lowered by some amount, provided the "demon" or the experimentalist who acts upon this system makes use of some amount of information at least equal to the decrease of the entropy. Conversely, in order to acquire some information, we need to raise the entropy of some system by a quantity at least equal to the amount of information gained. Information theory thus enlightens many aspects of statistical physics.

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13 References

- Abragam, A. and Goldman, M. (1982). *Nuclear magnetism: order and disorder* (pp. 45-49). Oxford: Clarendon.
- Allahverdyan, A.E., Balian, R. and Nieuwenhuizen, Th.M. (2003). Curie-Weiss model of the quantum measurement process. *Europhys. Lett.*, *61*, 452-458.
- Balian, R., Alhassid, Y. and Reinhardt, H. (1986). Dissipation in many-body systems: a geometric approach based on information theory. *Phys. Reports*, *131*, 1-146.
- Balian, R. and Balazs, N. (1987). Equiprobability, inference and entropy in quantum theory. *Ann. Phys. NY*, *179*, 97-144.
- Balian, R. (1989). On the principles of quantum mechanics. *Amer. J. Phys.*, *57*, 1019-1027.
- Balian, R. (1991 and 1992). *From microphysics to macrophysics: methods and applications of statistical physics* (vol. I and II). Heidelberg: Springer.
- Balian, R. (1999). Incomplete descriptions and relevant entropies. *Amer. J. Phys.*, *67*, 1078-1090, and references therein.

- Balian, R. (2004). Entropy, a protean concept. Poincaré seminar. *Progress in Math. Phys.* (pp. 119-144). Basel: Birkhäuser.
- Brillouin, L. (1956). *Science and information theory*. New York: Academic Press.
- Callen, H.B. (1975). *Thermodynamics*. New York: Wiley.
- Cox, R.T. (1946). Probability, frequency and reasonable expectation. *Amer. J. Phys.*, *14*, 1-13.
- de Finetti, B. (1974). *Theory of probability*. New York: Wiley.
- Greenberger, D., Horne, M., Shimony, A. and Zeilinger, A. (1990). Bell's theorem without inequalities. *Amer. J. Phys.*, *58*, 1131-1143.
- Jaynes, E.T. (1957). Information theory and statistical mechanics. *Phys. Rev.*, *106*, 620-630 and *108*, 171-190.
- Lieb, E.H. (1976). The stability of matter. *Rev. Mod. Phys.*, *48*, 553-569.
- Mayer, J.E. and Mayer, M.G. (1977). *Statistical mechanics* (second edition, pp. 145-154). New York: Wiley.
- Ruelle, D. (1969). *Statistical mechanics: rigorous results*. Reading: Benjamin.
- Shannon, C.E. and Weaver, W. (1949). *The mathematical theory of communication*. Urbana: University of Illinois Press.
- Thirring, W. (1981). *Quantum mechanics of atoms and molecules*. New York: Springer.
- Thirring, W. (1983). *Quantum mechanics of large systems*. New York: Springer.
- Uffink, J. (1995). Can the maximum entropy principle be explained as a consistency requirement? *Studies in Hist. and Philos. of Mod. Phys.*, *26B*, 223-261, and references therein.
- van Kampen, N.G. (1984). The Gibbs paradox. In W.E. Parry (ed.), *Essays in theoretical physics in honour of Dirk ter Haar* (pp. 303-312). Oxford: Pergamon.