



Prolegomena to a Non-equilibrium Quantum Statistical Mechanics

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Abstract—We suggest that the framework of quantum information theory, which has been developing rapidly in recent years due to intense activity in quantum computation and quantum communication, is a reasonable starting point to study non-equilibrium quantum statistical phenomena. As an application, we discuss the non-equilibrium quantum thermodynamics of black hole formation and evaporation.
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1. INTRODUCTION

The classical statistical theory of thermodynamical phenomena, due largely to Boltzmann, Maxwell, and Gibbs, is one of the cornerstones of 20th century physics. It describes equilibrium phenomena ranging from gas dynamics over steam engines to crystals, while its quantum extension accurately describes radiation phenomena, metals, and superconductivity, to name but a few examples. Nature's tendency to move towards equilibrium following a perturbation—captured by Boltzmann's second law—implies that most everyday-life phenomena are indeed taking place in an equilibrated system, for which this theory is applicable and eminently successful. For the brief *transitory* periods, however, the time during which a system *approaches* equilibrium, our bag of tricks—containing the tools of statistical mechanics—is of little use. The canonical phenomena of this type are relaxation or transport processes, phenomena which are usually termed “irreversible”, and phase transitions for which the entropy is not a constant.

The standard approach to deal with such situations is to study the N -body dynamics of the system, with a Hamiltonian that includes an interaction term (in equilibrium statistical mechanics the Hamiltonian is a sum of non-interacting one-body terms) and the construction of equations that follow the N -particle distribution function through time: the Boltzmann equation (see, e.g., [1]). This approach suffers from the drawback that it can only be solved in perturbation theory, which obscures the relation to the “exact” formalism of thermodynamics. In this paper, we would like to explore the possibility that a formalism well-known from engineering—Shannon's statistical theory of information—provides a bridge between equilibrium and non-equilibrium statistical phenomena, and that its quantum extension (developed primarily in support of the recent efforts in quantum computation and communication) represents an adequate framework to investigate certain quantum statistical phenomena that have so far resisted a satisfying treatment. Naturally, however, we should not expect that the classical and quantum theory of information provides a complete theory of all non-equilibrium phenomena. For most dynamics with complicated time-dependent interactions and many-body correlations, a transport-equation approach will still be the only tractable alternative.

Standard non-equilibrium phenomena are usually termed “irreversible”, an adjective that captures a practical aspect—a direction of time—which, however, we know not to be fundamental.

Rather, time-reversal invariance guarantees that all dynamics can, in principle, be reversed as long as the participating degrees of freedom can be controlled. Even though this is clearly not always possible in practice, it may appear as an oversight that a practical limitation seems to be at the origin of a theorem—the second law of thermodynamics. Indeed, as irreversibility is only practical, so must be the second law. If we were, then, able to devise a formalism in which the second law is replaced by a *conservation law* for entropy (and in which case the second law would appear as a corollary) we may then be in possession of a formalism that can quantitatively describe even the *approach* to equilibrium and other non-equilibrium statistical phenomena. It is the purpose of this paper to point out that this formalism exists in the form of the classical theory of information, introduced by Shannon [2]. Its extension to the quantum regime (see, e.g., [3] and references therein) is particularly interesting as it consistently describes quantum unitary dynamics which dictates that the von Neumann entropy—the quantum extension of the Shannon entropy—is a *constant*.

In the next section we begin by describing the classical statistical theory of information in physical terms (as opposed to the more engineering-oriented approach given in most textbooks [4]). We then apply it to two classical non-equilibrium statistical processes—measurement, and equilibration of an ideal gas—to demonstrate the use of the formalism in physics. In Section 3 we formulate the quantum theory with special emphasis on those aspects that differ from the classical theory, and discuss the EPR paradox as an illustration. We present an application to black hole formation and evaporation—a quintessential non-equilibrium scenario—in Section 4. We close with conclusions and comments in Section 5. Readers familiar with the information-theoretic approach to classical and quantum statistical phenomena may skip directly ahead to Section 4.

2. CLASSICAL THEORY

The intimate relation between information theory and statistical mechanics has been pointed out earlier by Jaynes [5] in order to *justify* statistical mechanics via information theory. Here, we use information theory to *extend* statistical mechanics to the non-equilibrium regime.

The concept of entropy was introduced by Shannon with respect to *random variables*. For a random variable X that can take on values x_1, \dots, x_N with probabilities p_1, \dots, p_N respectively, the Shannon *uncertainty* (or entropy) is given by

$$H(X) = - \sum_{i=1}^N p_i \log p_i . \quad (1)$$

Instead of random variables, however, we may imagine any physical system with enumerable degrees of freedom and enumerable states x_i . As is well-known and we show below, the Shannon entropy then represents the *physical* entropy of the system. In fact, this concept of entropy can be expanded to cover continuous variables, where it will suffer from the same ambiguity (redefinition up to a constant) as standard thermodynamical entropy. For the moment, let us confine ourselves to discrete degrees of freedom and imagine that any continuous variables are *coarse-grained* (either by assuming appropriate boundary conditions, or else artificially.)

The relation to Boltzmann–Gibbs entropy becomes manifest if we consider not *general* probability distributions $\{p_i\}$, but an equilibrium distribution where the p_i are given by the Gibbs distribution:

$$p_i = \frac{1}{Z} e^{-E_i/kT} , \quad (2)$$

where E_i is the *energy* of state x_i , and p_i then represents the *probability* of X to take on energy E_i . Note that this probability is normalized by the partition function $Z = \sum_i e^{-E_i/kT}$. Inserting

(2) into eqn (1) produces

$$H = \frac{\langle E \rangle}{kT} + \log Z = \frac{1}{kT} (\langle E \rangle - F) \quad (3)$$

and confirms that the Shannon entropy is just the standard physical entropy in statistical mechanics and thermodynamics when rescaled by the Boltzmann constant k :

$$S = kH. \quad (4)$$

Above, we defined the free energy $F = -kT \log Z$ in the usual manner. Similarly, thermodynamical averages are obtained via

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^N A_i e^{-E_i/kT} \quad (5)$$

for an observable A that takes on the value A_i in state x_i .

Returning to random variables for a moment, imagine an additional variable Y that takes on states y_1, \dots, y_N with probabilities p'_1, \dots, p'_N . We can then define the conditional probability of finding X in state x_i , given that Y is in state j

$$p_{i|j} = \frac{p_{ij}}{p'_j}, \quad (6)$$

where p_{ij} is the *joint* probability to find X in state x_i and simultaneously Y in state y_j . This concept will allow us to quantify *correlations* between degrees of freedom, a particularly important task in non-equilibrium systems. Indeed, equilibrium can be *defined* as the state where “all ‘fast’ things have happened and all the ‘slow’ things not” [6], which implies that all non-permanent correlations have vanished in equilibrium.

Armed with conditional probabilities, we can define the *conditional entropy* of system X given that Y is in, say, state y_j , i.e., the entropy of X if we are fully aware that Y is in state y_j , or in other words, the *remaining* entropy of X if Y is held fixed in state y_j . Naturally, this is defined as

$$H(X|y_j) = - \sum_i p_{i|j} \log p_{i|j}. \quad (7)$$

Also, the *average conditional entropy* of X given Y is in *any* fixed state, or quite generally is *known*, is then

$$H(X|Y) = \langle H(X|y_j) \rangle = - \sum_{ij} p_{ij} \log p_{i|j}. \quad (8)$$

The vertical bar in the expression $H(X|Y)$ denotes the conditional nature of the entropy, and is usually read as “ X given Y ”, or “ X knowing Y ”.

Armed with the conditional (or remaining) entropy, we can find a measure for the amount of correlation between two systems. This is just the ordinary entropy minus the remaining entropy if one of the system’s variables are known: the *shared* entropy (also called correlation, or mutual, entropy)

$$H(X : Y) = H(X) - H(X|Y). \quad (9)$$

This is the central quantity introduced by Shannon: the mathematical measure of *information*[†]. The relation between unconditional (also called “marginal”) entropies such as $H(X)$ or $H(Y)$,

[†]The colon between X and Y is customarily used to indicate a shared entropy, and reminds us that correlation entropy is symmetric: $H(X : Y) = H(Y : X)$.

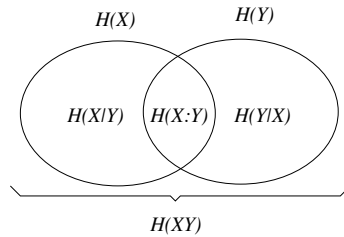


Fig. 1. Entropy Venn diagram for two random variables X and Y .

mutual, and conditional entropies are best visualized by *Venn diagrams*. In Fig. 1, the area of each circle represents an entropy, whereas the union of both circles represents the joint entropy $H(XY)$.

It is straightforward to see that these quantities can be translated into thermodynamics, by replacing the arbitrary probability distributions by equilibrium ones. We can see immediately, however, why they play no role in equilibrium thermodynamics. The probability of system X to take on energy E_i if Y has energy E_j is trivial: it is just given by $Z^{-1}e^{-E_i/kT}$ simply *because* X and Y are in equilibrium. Thus, in equilibrium, $H(X|Y) = H(X)$, and $H(X : Y) = 0$. Away from equilibrium, conditional and mutual *thermodynamical* entropies become crucial, as we now see.

2.1. Measurement

We first treat the dynamics of classical *measurement*. A measurement involves the contact between two equilibrated systems, usually at different temperatures. The measurement device is constructed in such a manner as to induce correlations between some of its variables—the “pointer”—and the measured system’s degrees of freedom (those which we desire to measure). After the initial contact between the systems and subsequent relaxation, equilibrium is re-established but thermodynamics seems to offer a paradox: the entropy of the measured system appears to have been reduced. Furthermore, this reduced entropy *can* be used to perform work—in apparent violation of the second law (this puzzle is usually termed the *Maxwell demon* paradox, see, e.g., [7]). While this dynamics is again practically irreversible, we can describe what happens in terms of the entropies introduced above.

Before the measurement, the system (denoted by S) is independent of the measurement device (denoted by M , see Fig.2a). They do not share any entropy, which implies that knowledge of any one of the systems will not allow any predictions about the other. Bringing the two systems into contact introduces correlations, and reduces the *conditional* entropy of both S and M . Note that before measurement, $H(S|M) \equiv H(S)$. The amount by which the conditional entropy is reduced is of course just the *acquired information*, or shared entropy $H(S : M)$ (see Fig. 2b). This shared entropy plays a fundamental thermodynamical role: for example it can be shown that erasing it requires the dissipation of an equal amount of heat [8]. Needless to say, the marginal entropy did not really decrease in this process, but rather *stayed constant*. In contrast, the conditional entropy of S is reduced, as can be seen by inspection of the diagram in Fig. 2b,

$$H(S) \longrightarrow H(S|M) = H(S) - H(S : M) . \quad (10)$$

Turning eqn (10) around:

$$H(S) = H(S|M) + H(S : M) \quad (11)$$

demonstrates that non-equilibrium dynamics affects only the distribution of $H(S)$ into either (conditional) entropy or information, that the two however always add up to $H(S)$.

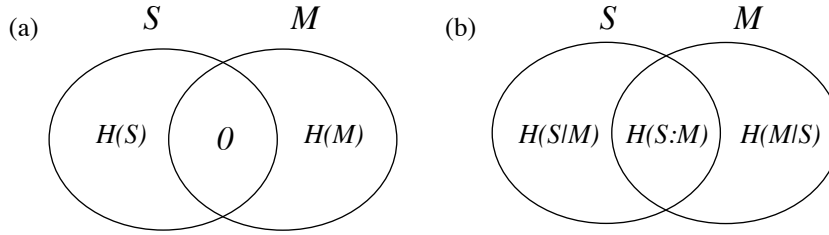


Fig. 2. Rearrangement of entropies in the measurement process. (a) System S and device M are uncorrelated ($H(S : M) = 0$). (b) Device and system share entropy $H(S : M)$ and the conditional entropy of both system and device are reduced.

2.2. Equilibration

Another example of irreversible dynamics is the notorious “perfume bottle” experiment, in which a diffusive substance (let’s say, an ideal gas) is allowed to escape from a small container into a larger one. Both the initial and the final state of the system is in equilibrium; common wisdom however states that the entropy of the gas is *increasing* during the process, reflecting the non-equilibrium dynamics. We shall now show that this is not the case, by describing the gas in the smaller container by a set of variables A_1, \dots, A_n , one for each molecule. The entropy $H(A_i)$ thus represents the entropy per molecule. The entire volume, on the other hand, is described by the *joint entropy*

$$H_{\text{gas}} = H(A_1 \cdots A_n), \quad (12)$$

which can be much smaller than the sum of per-particle entropies, the standard (equilibrium) thermodynamical entropy S_{eq}

$$H(A_1 \cdots A_n) \ll \sum_{i=1}^n H(A_i) = S_{\text{eq}}. \quad (13)$$

The difference is given by the n -body correlation entropy

$$H_{\text{corr}} = \sum_{i=1}^n H(A_i) - H(A_1 \cdots A_n) \quad (14)$$

which can be calculated in principle, but becomes cumbersome already for more than three particles.

We see that in this description the molecules after occupying the larger volume cannot be independent of each other, as their locations are *in principle* correlated (as they all used to occupy a smaller volume, see Fig. 3a). These correlations are not manifest in two- or even three-body correlations, but are complicated n -body correlations which imply that their positions are not independent, but linked by the fact that they share initial conditions. Again, this state of affairs can be summarized by turning around eqn (14)

$$H(A_1 \cdots A_n) = \sum_{i=1}^n H(A_i) - H_{\text{corr}}. \quad (15)$$

We assume that before the molecules are allowed to escape, they are uncorrelated with respect to each other: $H_{\text{corr}} = 0$, and all the entropy is given by the extensive sum of the per-molecule entropies. After expansion into the larger volume, the standard entropy increases because of the increase in available phase space, but this increase is balanced by an increase in the correlation entropy H_{corr} in such a manner that the actual joint entropy of the gas, H_{gas} , remains unchanged.

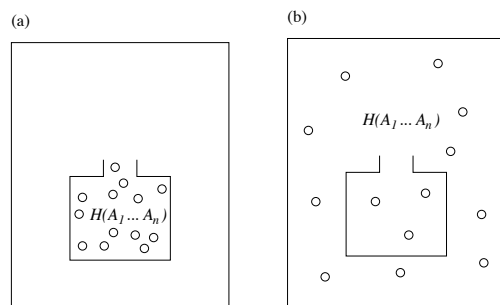


Fig. 3. Diffusion of an ideal gas from a small into a larger container. (a) The molecules with entropy $H(A_1 \dots A_n)$ occupy the smaller volume, and their correlation entropy is zero. (b) The molecules have escaped into the larger container, which increases the sum of the per-particle entropies and increases the correlation entropy commensurately such that the overall entropy remains unchanged.

Note that this description is not, strictly speaking, a redefinition of thermodynamical entropy. While in the standard theory entropy is an *extensive*, i.e., additive quantity for uncorrelated systems, the concept of a thermodynamical entropy in the absence of equilibrium distributions has been formulated as the number of ways to realize a given set of occupation numbers of states of the joint system (which gives rise to (1) by use of Stirling's approximation, see, e.g., [9]) and is thus fundamentally *non-extensive*. Assuming the systems A_i are uncorrelated reduces $H(A_1 \dots A_n)$ to the extensive sum $\sum_{i=1}^n H(A_i)$, and thus to an entropy proportional to the volume the systems inhabit. From a calculational point of view the present formalism does not represent a great advantage in this case, as the correlation entropy H_{corr} can only be obtained in special situations, when only few-body correlations are important.

The examples of non-equilibrium processes treated here (measurement and equilibration) suggest that:

In a thermodynamical equilibrium or non-equilibrium process, the unconditional (joint) entropy of a closed system remains a constant.

This formulation of the second law directly reflects probability conservation (in the sense of the Liouville theorem), and allows a quantitative description of the amount by which the conditional entropy is decreased in a measurement, or the amount of per-particle entropy is increased in an equilibration process.

3. QUANTUM THEORY

As the classical non-equilibrium mechanics described above is founded on the classical theory of information, its quantum extension is built on the quantum theory of information introduced recently [10–12].

3.1. Equilibrium

For our purposes, equilibrium quantum statistical mechanics can be summarized in a few equations. For a system described by Hamiltonian[†] H and partition function (we set $\beta = 1/kT$ from now on)

$$Z = \text{Tr} e^{-\beta H}, \quad (16)$$

[†]In the following, H stands for the Hamiltonian, while entropies are denoted by the symbol S .

the density matrix can be written as

$$\varrho = \frac{e^{-\beta H}}{Z} \quad (17)$$

while the free energy is

$$F = -\frac{1}{\beta} \log Z. \quad (18)$$

Accordingly,

$$\log \varrho = \beta F - \beta H \quad (19)$$

and, defining the internal energy $U = \text{Tr } \varrho H$, we obtain the equivalent of eqn (3)

$$S = \beta(U - F) \quad (20)$$

where

$$S(\varrho) = -\text{Tr } \varrho \log \varrho. \quad (21)$$

is the quantum entropy of the state described by the density matrix ϱ , introduced by von Neumann [13]. While we used equilibrium expressions to motivate (21), it is in fact valid even when an equilibrium expression such as (17) does not exist. Just as the classical entropy (12), this entropy remains a constant under *any* dynamics, reversible or irreversible. This is in fact more obvious in the quantum case, as the density matrix ϱ is known to evolve in a unitary manner

$$\varrho(t) = U(t)\varrho(0)U^\dagger(t) \quad (22)$$

which immediately implies, using (21) and the cyclic property of the trace, that

$$\frac{d}{dt} S(t) = 0. \quad (23)$$

Inserting (17) into (21) on the other hand allows us to recover the Boltzmann–Gibbs–Shannon entropy (1), with the probabilities given by

$$p_i = \frac{1}{Z} e^{-\beta E_i} \quad (24)$$

with E_i the eigenvalues of H . In general, when considering the diagonal elements of ϱ in a basis distinct from the eigenbasis of H , the von Neumann entropy is a lower bound on the Boltzmann–Gibbs–Shannon entropy

$$S(\varrho) \leq -\sum_i p_i \log p_i, \quad (25)$$

where the equality holds for density matrices ϱ that are diagonal, in which case quantum statistical mechanics is formally identical to the classical description. Differences arise for non-diagonal ϱ . The off-diagonal terms signal the presence of quantum *superpositions* and the potential for *entanglement*—a form of “super-correlation”. As we shall see, entanglement requires a radical departure from the classical description, and an extension of the above formalism to a non-equilibrium quantum statistical mechanics.

3.2. Non-equilibrium

As mentioned earlier, in classical mechanics equilibrium between two ensembles A and B implies that all “fast” degrees of freedom are independent (no correlations) whereas the “slow” degrees are considered to be static. This is usually achieved by waiting for times larger than the relaxation time. The situation is dramatically different in quantum mechanics. As we shall see, entanglement introduces a type of super-correlation that cannot be undone by letting the system equilibrate, not even if the two systems are separated by space-like distances.

As an example, consider the joint system AB where A and B are half-integral spin states with eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$. It is then possible to construct a wavefunction for the joint system AB which makes it mathematically and logically impossible to attribute a *state* to either A or B by itself: the well-known EPR state

$$|\Psi_{AB}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) . \quad (26)$$

However, both A and B can be described by *reduced* density matrices, obtained by tracing B or A out of the joint matrix ϱ_{AB}

$$\varrho_{A(B)} = \text{Tr}_{B(A)} \varrho_{AB} = \frac{1}{2} \left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \right) , \quad (27)$$

where $\text{Tr}_{B(A)}$ denotes the partial trace over $B(A)$. As these density matrices are diagonal, the quantum entropy is just equal to the classical one

$$S(A) = S(B) = 1 \quad (28)$$

if we agree to take base-2 logarithms and count entropy in “bits”. The joint entropy $S(AB)$ on the other hand is *not* equal to 2, i.e., the entropy is *non-extensive*. As we mentioned earlier, this implies that correlations are present and calls for a non-equilibrium formalism. Things are worse here. For this wavefunction, the quantum entropy *vanishes* (it is a pure state: the only non-vanishing eigenvalue of the density matrix $\varrho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$ is 1.) This well-known property of quantum mechanically entangled systems is known as the *non-monotonicity* of quantum entropy (see, e.g., [14]) and forces us to rethink the equilibrium formalism that we recapitulated earlier. We will proceed in a manner similar to the non-equilibrium classical mechanics of the previous section, by introducing quantum *conditional* and *mutual* entropies. As in the classical case, the conditional quantum entropy then would reveal to us the entropy of a quantum system *given* we know the state of another system it is entangled with, while the quantum mutual entropy would reflect the amount of correlation between the systems. In contrast to the classical situation, quantum conditional entropies can be *negative*, while the mutual entropy can *exceed* the classically allowed limit (hence the term super-correlation.) This formalism has turned out to be useful in the information-theoretic analysis of quantum measurement [12,15], as well as the description of the non-equilibrium physics of quantum information transmission [16].

Guided by the classical case, we are tempted to define the conditional quantum entropy of system A given the state of B by

$$S(A|B) = S(AB) - S(B) , \quad (29)$$

i.e., the quantum entropy of the joint system minus the entropy of B (as that is given). This structure then suggests an expression for the *conditional amplitude matrix* $\varrho_{A|B}$, which we need to formulate the non-equilibrium dynamics. This matrix, first introduced in [11], is a well-defined Hermitian operator on the joint Hilbert space of A and B (see [17]) defined by

$$\varrho_{A|B} = \exp[\log \varrho_{AB} - \log(\mathbf{1}_A \otimes \varrho_B)] \quad (30)$$

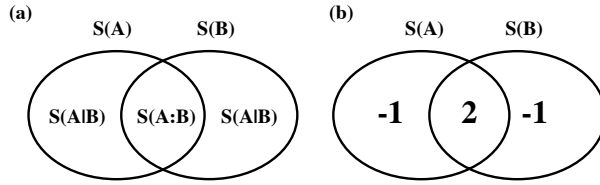


Fig. 4. Quantum entropy Venn diagrams. (a) Definition of joint $[S(AB)]$ (the total area), marginal $[S(A)$ or $S(B)]$, conditional $[S(A|B)$ or $S(B|A)]$ and mutual $[S(A : B)]$ entropies for a quantum system AB separated into two subsystems A and B ; (b) their respective values for the EPR pair.

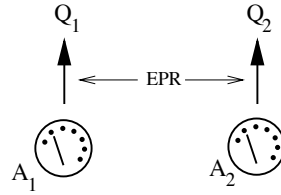


Fig. 5. Measurement of EPR pair Q_1Q_2 by devices A_1 and A_2 .

which allows us to write

$$S(A|B) = -\text{Tr} \varrho_{AB} \log \varrho_{A|B} \tag{31}$$

in analogy with (8). In contrast to the classical conditional probability $p_{i|j}$, the conditional amplitude matrix can have eigenvalues *exceeding* unity, which reflect the quantum inseparability of the system.

The mutual quantum entropy can be defined in an analogous manner

$$S(A : B) = S(A) - S(A|B) \tag{32}$$

as the marginal (unconditional) quantum entropy of A minus the “remaining” entropy $S(A|B)$. Consequently, we can extend the useful Venn diagram technique (Fig. 1) to the quantum regime, and just replace H by S (Fig. 4a). The peculiarity of quantum superpositions such as the EPR wavefunction eqn (26) is immediately apparent in its Venn diagram (Fig. 4b).

More generally, a mixed state $\varrho = \sum_i p_i |i\rangle\langle i|$ can always be “purified”, i.e., written as the partial trace over a pure state $|\psi\rangle = \sum_i \sqrt{p_i} |i\rangle|i\rangle$ by means of the Schmidt decomposition, while being represented by a Venn diagram such as Fig. 4b but with entries $\{-S, 2S, -S\}$ instead of $\{-1, 2, -1\}$, where $S = -\sum_i p_i \log p_i$. Furthermore, the diagram technique and the use of quantum entropies can easily be extended to understand the quantum correlations between three systems. An instructive example is the description of the EPR paradox [18], which we briefly summarize as it is relevant to the discussion of black holes which follows.

Imagine a wavefunction such as (26), with the particles in question separated by space-like distances. Imagine further that at each of these separated locations, measurements of the spin-projection are performed in either the x or the z direction. Beyond the quantum bipartite system described by eqn (26), which we denote by Q_1Q_2 in the following, we introduce Hilbert spaces for the measurement devices, the “ancillae” A_1 and A_2 rigged to measure the polarization of Q_1 and Q_2 respectively (see Fig. 5). Depending on whether same (Fig. 6) or orthogonal (Fig. 7) polarizations are measured at the remote locations, the measurement devices are either correlated or independent. However, in both cases, the entanglement between quantum systems and measurement devices is more complicated, and even in case the measurement devices appear uncorrelated (Fig. 7b), subtle entanglement persists.

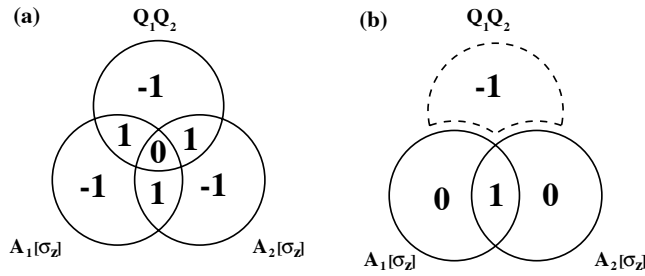


Fig. 6. (a) Quantum entropy diagram for the EPR measurement of same spin-projections: e.g., A_1 and A_2 both measure σ_z . (b) Reduced diagram obtained by tracing over the quantum states Q_1 and Q_2 (the dashed line surrounds degrees of freedom traced out, i.e., averaged over) reflecting the correlation between the measurement devices.

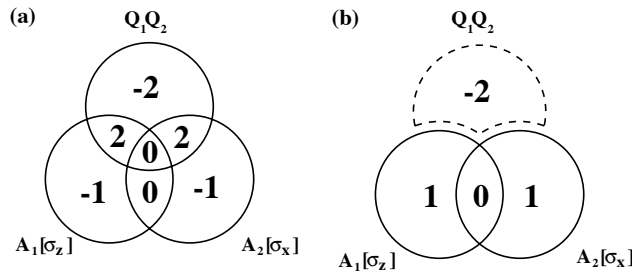


Fig. 7. (a) Quantum entropy diagram for the EPR measurement of orthogonal spin-projections, e.g., A_1 measures σ_z while A_2 records σ_x . (b) Reduced diagram as above. In this case the measurement devices show zero correlation, while entanglement persists between quantum system and measurement devices.

4. BLACK HOLE FORMATION AND EVAPORATION

The discovery of Hawking radiation [19] appears to have plunged quantum mechanics into a deep crisis, as it seems to imply that the evaporation of black holes violates unitarity (for a review, see, e.g., [20]). Below, we formulate the “information-loss” problem in terms of the formalism described here, and argue for a consistent description in terms of quantum non-equilibrium thermodynamics.

4.1. Black hole entropy and information paradox

Black holes have the remarkable property that they are fully described by very few variables—a non-rotating non-charged black hole by only one, its mass. Bekenstein [21] and Hawking [19] determined that an *entropy* can be defined for a Schwarzschild black hole which is given entirely in terms of the area A inside the event horizon

$$S_{BH} = \frac{1}{4}A. \tag{33}$$

This area, in turn, is just $A = 4\pi R^2$ where R is the radius of the black hole given (in units where $\hbar = G = 1$) by $R = 2M$, so that the black hole entropy is specified entirely in terms of the black hole mass M

$$S_{BH} = 4\pi M^2. \tag{34}$$

While a number of reasonings lead to this expression, including the counting of microscopic quantum states that give rise to a black hole, Hawking [22] pointed out that the process of

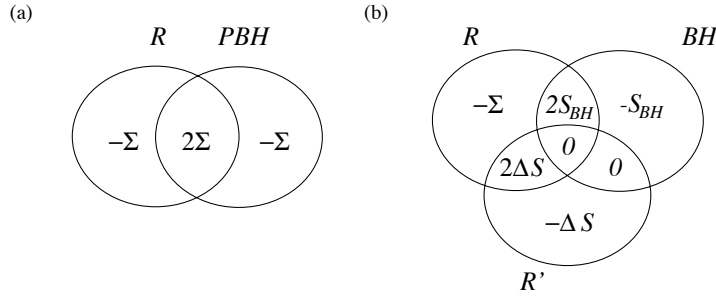


Fig. 8. Venn diagrams for black hole formation. (a) Just before collapse. (b) After collapse. Σ denotes the entropy of the proto-black-hole, while S_{BH} is the Bekenstein-Hawking entropy, and ΔS is the entropy deficit.

thermal evaporation of a black hole leads to an “information paradox”. If we assume that the black hole is formed from a quantum mechanically pure state $S = 0$, the entropy of the purely thermal blackbody radiation left behind *after evaporation* should be of the order $\sim M^2$, i.e., a pure state evolved to a mixed one. This contradicts the unitary evolution of quantum states eqn (22), according to which (as we have pointed out repeatedly) the entropy of a closed system is a constant, in this particular case the constant zero.

Several avenues have been proposed to escape this conclusion, and we will focus here on the most conservative explanation, namely that Hawking radiation is effectively *non-thermal* (in the sense that quantum correlations between the radiation and the state of the black hole exist in principle), and that a pure state *is* formed after evaporation, only that it is impossible to distinguish it from purity [23–25]. We first note that beyond the information paradox pointed out by Hawking, as observed by Zurek [26] we also need to match the black hole entropy S_{BH} with the entropy of approximately thermal radiation $S_{\text{rad}} \sim T_H^3$ with black hole temperature $T_H = (8\pi M)^{-1}$. We then proceed to propose a scenario in which this might be achieved.

4.2. Black hole formation from a pure state

Of course, black holes do not form by the “collapse” of a pure state. Rather, we can imagine that part of a pure state with marginal entropy $S_{\text{rad}} \equiv \Sigma$ disappears behind an event horizon. Let us divide space just before the collapse into a region PBH (the proto-black-hole) and R , the remainder. As the entire system is pure ($S = 0$), we know that $S_{\text{rad}} = S_{PBH}$. The entropy diagram for this situation can be constructed as described in the previous section, and is shown in Fig. 8a.

The degrees of freedom in R are practically inaccessible after the collapse of the region PBH , but we should keep in mind that they are *entangled* with PBH in such a manner that the entire system, (R, PBH) , is pure. In the language of quantum information theory, R is a “reference” system that “purifies” PBH . The gravitational collapse of region PBH forms an intriguing problem. While we can assume the radiation inside it to be purely thermal, with energy $E \sim T^4$ and corresponding entropy $\Sigma \sim 4/3 T^3$, the entropy of the *collapsed* state is $S_{BH} = 4\pi M^2$, lower than Σ . In fact, it was shown by Zurek [26] that the entropy dS accreted by a black hole (which we can take to be of the radiation type) is larger than the corresponding entropy increase of the black hole itself

$$dS \approx 4/3 dS_{BH} , \tag{35}$$

and the same mismatch occurs in the evaporation process.

In statistical physics this is not an alarming state of affairs, but rather is the usual scenario in a non-equilibrium phase transition. Here, we shall mask our ignorance about the dynamics which

produces the black hole out of radiation by assigning a new *phase* to the black hole matter, and discuss the process in which the radiation with entropy Σ *condenses* to a phase with entropy S_{BH} .

During the condensation from the proto-black-hole state to the black-hole (*BH*) state, excess entropy ΔS has to be radiated away ($T_H \Delta S$ is the equivalent of the latent heat in a first-order phase transition). While we cannot offer a detailed picture of this transition, we assume that this radiation is emitted just outside the forming horizon, and represents the bremsstrahlung of the accelerated particles accreting on the black hole. This gives rise, then, to the system depicted in Fig. 4b, where the bremsstrahlung R' is entangled with both R and the black hole BH , with marginal entropy $S(R') = \Delta S = \Sigma - S_{BH}$. During the phase transition, the entropy of the *PBH* system remains constant, but is distributed over the joint system (BH, R'):

$$\Sigma = S(PBH) = S(R', BH) = S(BH) + S(R'|BH) = S_{BH} + \Delta S. \quad (36)$$

The “missing” entropy ΔS therefore is contained in radiation R' emitted during the collapse.

This scenario, which is the time-reverse of the evaporation process considered next, naturally leads to a radiation field R' that is causally uncoupled from the black hole, as $S(BH : R') = 0$. Tracing over the “reference” field R leads to the trivial entropy diagram $\{S_{BH}, 0, \Delta S\}$. We need to keep in mind, however, that just as in the EPR situation described previously, the wavefunctions of R' and the black hole are linked via entanglement with the quantum degrees of freedom R .

4.3. Evaporation of black holes

The processes of black hole formation and evaporation can be considered time-reverse images of each other. Evaporation of black holes occurs through the formation of virtual particle–anti-particle pairs of energy $2dE$ close to the horizon due to quantum mechanical tunneling in the strong gravitational field. If one of the members of the pair disappears behind the horizon while the other manages to escape, the escaping particle appears to have a black-body spectrum with temperature T_H , while the energy of the black hole is reduced by dE . The paradox occurring here thus appears to be the same as the one encountered in the condensation process. How does the radiation pick up the extra entropy? In terms of quantum information theory, the creation of a particle–anti-particle pair is akin to the creation of an EPR state with vanishing entropy, described by the entropy diagram in Fig. 4b. However, just as in standard first-order “evaporation” transitions, the black hole has to provide in addition the latent heat for “decondensation”, i.e., the energy to create the entropy ΔS . Thus, a pair created with $2dE$ and temperature T_H will not reduce the black hole mass by an amount dE , but by

$$\Delta E = dE - T_H \Delta S, \quad (37)$$

which restores the entropy and energy balance. The entropy of the escaping particle is $dS \sim T_H^3$ while at the same time the entropy of the black hole is reduced by

$$dS_{BH} = 4\pi \left(M^2 - (M - \Delta E)^2 \right) = \frac{dE}{T_H} - \Delta S. \quad (38)$$

Arguments have been raised (see the reviews [20] and in particular [27]) that seem to imply that information stored in correlations and entanglement between the black hole and its surrounding radiation field cannot be retrieved, even in principle. These arguments rest on the assumption that the (low-energy) quantum fields live in a Hilbert space that is of the product form $\mathbf{H}_{in} \otimes \mathbf{H}_{out}$, and an application of the quantum no-cloning theorem. While the fields do live in a product Hilbert space, the wavefunction of an EPR pair created at the event horizon of the black hole indirectly becomes entangled with the hole the moment one of the particles crosses the horizon (even

though the quantum fields are separated by space-like distances) and the combined quantum state becomes inseparable. This situation is not unlike the scenario we noted in the formation of the black hole, where the accreted particle and the radiation it emits when tumbling into the black hole can be considered an entangled, EPR-type state (albeit with real rather than virtual energy). Just as in that case the radiation R' shared no entropy with the black hole, neither does the Hawking radiation, while still being entangled with it. Thus, the Hawking radiation carries “information” about the inside of the hole in the same manner as the measurement of EPR partners separated by space-like distances reveals correlations in measurement devices that are at space-like distances. Yet, a fundamental problem remains that is unlikely to be solved within the present formalism. The Hawking radiation—while emitted in a unitary manner and while information loss certainly does not take place—remains causally uncorrelated to the black hole as long as the horizon separates the black hole entropy from the radiation field. In a sense, we have to wait until the last moment—the disappearance of the black hole—for the entropy balance to be restored. This appears to put a severe strain on current black hole models, as it is hard to imagine that this much entropy can be stored in an ever-shrinking black hole. This problem is likely due to our incomplete understanding of late-stage black holes, rather than a problem intrinsic to quantum mechanics.

An alternative solution would present itself if the Bekenstein-Hawking entropy could be understood in terms of a *conditional* entropy. In that case, entropy flow from the black hole to the outside via the formation of virtual pairs is understood easily, as the member of the pair that crosses the horizon not only has negative energy but also negative conditional entropy (see Fig. 4b). As a conditional entropy can become as negative as the marginal entropy of the system it is a part of, we can circumvent the argument that “the black hole cannot store the information until the end because it runs out of quantum states”, because the radiation could “borrow” as much entropy as necessary from the black hole until the horizon has disappeared. Within the present framework, there appears to be no physical picture which would suggest that the Bekenstein-Hawking entropy is in fact conditional. It is not inconceivable, however, that a quantum statistical information theory extended to curved space-time would reveal such a state of affairs.

5. CONCLUSIONS

We have used a formalism developed in the exploration of quantum computers—quantum information theory—to describe quantum processes away from thermodynamical equilibrium, such as the formation and evaporation of black holes. The formalism emphasizes the *conservation* of entropy, and is particularly useful in situations where entropy is distributed over two or three systems. We emphasize that great care is needed in using the concepts of entropy and information consistently: information, for example, can *never* be “stored” in one system (e.g., a black hole). Rather, information is a measure of correlation *between* two systems, which implies that information is *always* stored in correlations. The analysis of information storage in black hole formation and evaporation presented here is a simple application of these rules to a scenario in which black holes are considered special states of matter with an equation of state different from that of radiation (or usual matter). Transitions between those states occur continuously as the specific heat of black hole matter is negative [19]. As a consequence, radiation and black hole matter are unstable at any time, and transitions must occur as long as matter of either kind is present. Yet, a consistent formulation of the correlations between radiation and matter shows that entropy is not created during the process, and consequently that information is conserved. Still, the mechanism by which the pure state is restored in the last stages of black hole evaporation may require deeper insights into quantum gravitational dynamics, and possibly an extension of

information theory to curved space-time.

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