COLLAPSE OF THE ENTANGLED STATE AND THE
ENTROPY INCREASE IN AN ISOLATED SYSTEM *

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Abstract

We show that the collapse of the entangled quantum state makes the entropy increase in
an isolated system. The second law of thermodynamics is thus proven in its most general
form.
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To understand the foundation of the second law of thermodynamics is a long standing prob-
lem in physics. The H-theorem of Boltzmann is a classical proof of the law. It is based on a
model of colliding classical particle system for the macroscopic matter, therefore is not general
enough, even from the view point of the classical statistical physics. Here we show an informa-
tion theoretical proof of the law. It is based on the state entanglement in time development and
the state collapse in measurement, therefore is quite general.

The time development of the density operator $\rho(t)$ for an isolated system is governed by the
von Neumann equation. Its solution is

$$\rho(t) = U(t,t_0)\rho(t_0)U(t_0,t) ,$$

in which $U(t,t_0)$ is the time displacement operator of the state from time $t_0$ to time $t$. Defining
the information

$$I(t) = \text{Tr}[\rho(t)\ln\rho(t)]$$

at time $t$, we see from (1)

$$I(t) = \text{Tr}[U(t,t_0)\rho(t_0)\ln\rho(t_0)U(t_0,t)] = \text{Tr}[\rho(t_0)\ln\rho(t_0)U(t_0,t)U(t,t_0)] = I(t_0) ,$$

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because of $U(t_0, t)U(t_0) = 1$. It is the information conservation in quantum mechanics.

To measure the entropy of a system, one has to divide the system into macroscopically infinitesimal parts. The entropy of the $i$th part is defined to be $S_i = -k_B \text{Tr}(\rho_i \ln \rho_i)$, in which $\rho_i$ is the reduced density operator of the part $i$. The entropy of the whole system is defined to be the sum

$$S = \sum_i S_i = -k_B \sum_i \text{Tr}(\rho_i \ln \rho_i)$$

(4)

of the entropies of these parts, as an extensive thermodynamical variable should be. When one measures the entropy of the system at time $t_0$, he has destroyed the entanglement of the states of various parts of the system. The state and the density operator of the system are therefore factorized. Under this condition, the entropy of the system is

$$S(t_0) = -k_B \sum_i \text{Tr}[\rho_i(t_0) \ln \rho_i(t_0)] = -k_B \text{Tr}[\rho(t_0) \ln \rho(t_0)] = -k_B I(t_0) .$$

(5)

For an isolated system, the information conservation (3) works. The information of the system at $t > t_0$ is therefore

$$I(t) = -S(t_0)/k_B .$$

(6)

During the period from time $t_0$ to $t$, the interaction between different parts of the system makes their states be entangled again. It means the states of different parts are correlated. If one measures the entropy of the system at time $t$, he has to measure the entropies of every part of the system, and therefore destroy this entanglement once more. This is the state collapse, and causes the loss of correlation information. Since the parts of the system are not isolated, their information is not conserved. It makes the entropy

$$S(t) = -k_B \sum_i \text{Tr}[\rho_i(t) \ln \rho_i(t)]$$

(7)

at time $t$ does not equal $S(t_0)$ in general. By intuition we see, the sum of information of all parts of the system should not be more than the information of the system, since the correlation information of various parts is not included in the sum. It is

$$\sum_i \text{Tr}[\rho_i(t) \ln \rho_i(t)] \leq I(t) .$$

(8)

If this is true, we obtain

$$S(t) \geq S(t_0)$$

(9)

from (6)-(8) for an isolated system. This is exactly the second law of thermodynamics.

To prove the statement (8), let us remind you the following mathematical inequalities. To make this paper be self-contained, we also collect the proofs of these inequalities here, although they may be found in text books.

Lemma 1. For any positive number $x$ we have

$$x \ln x \geq x - 1 ,$$

(10)
the equality holds when and only when $x = 1$.

Proof: It may be verified by differentiation, that $x \ln x - (x - 1)$ as a function of positive variable $x$ has unique minimum $0$ at $x = 1$. The lemma is therefore proven.

Lemma 2. For set $[w_i]$ of positive numbers and set $[x_i]$ of non-negative numbers with $\sum_i x_i = 1$, we have

$$\sum_i x_i w_i \ln \sum_i x_i w_i \leq \sum_i x_i w_i \ln w_i .$$  \hspace{1cm} (11)

Proof: The average $\bar{w} \equiv \sum_i x_i w_i$ is positive. By lemma 1 we see

$$\sum_i x_i w_i \ln \sum_i x_i w_i - \sum_i x_i w_i \ln w_i = \sum_i x_i w_i \ln \frac{\bar{w}}{w_i}$$
$$= - \sum_i x_i \bar{w} \frac{w_i}{\bar{w}} \ln \frac{w_i}{\bar{w}} \leq - \sum_i x_i \bar{w} \left( \frac{w_i}{\bar{w}} - 1 \right) = 0 .$$

The lemma is therefore proven.

Lemma 3. For set $[W_i]$ of positive numbers and set $[T_{ij}]$ of non-negative numbers with

$$\sum_i W_i = 1 \quad \text{and} \quad \sum_i T_{ij} = \sum_j T_{ij} = 1 ,$$  \hspace{1cm} (12)

we have

$$W_j' \equiv \sum_i W_i T_{ij} > 0 \quad \text{for every } j,$$  \hspace{1cm} (13)

$$\sum_j W_j' = 1 ,$$  \hspace{1cm} (14)

and

$$\sum_j W_j' \ln W_j' \leq \sum_i W_i \ln W_i .$$  \hspace{1cm} (15)

Proof: (13) and (14) are obvious. By (12) and lemma 2 we see

$$\sum_j W_j' \ln W_j' = \sum_j \left( \sum_i W_i T_{ij} \right) \ln \left( \sum_i W_i T_{ij} \right) \leq \sum_i W_i T_{ij} \ln W_i = \sum_i W_i \ln W_i .$$

The lemma is therefore proven.

Lemma 4. For positive numbers $[W_{ij}]$, $W_i = \sum_j W_{ij}$ and $W_j' = \sum_i W_{ij}$, with $\sum_{ij} W_{ij} = 1$, we have

$$\sum_i W_i = 1 , \quad \sum_j W_j' = 1 ,$$  \hspace{1cm} (16)

and

$$\sum_{ij} W_{ij} \ln W_{ij} \geq \sum_i W_i \ln W_i + \sum_j W_j' \ln W_j' .$$  \hspace{1cm} (17)

The equality holds when and only when $W_{ij} = W_i W_j'$ for all $ij$, it is that the $W_{ij}$ may be factorized.
Proof: (16) is obvious. By lemma 1 we see
\[ \frac{W_{ij}}{W_i W_j} \ln \frac{W_{ij}}{W_i W_j} \geq \frac{W_{ij}}{W_i W_j} - 1, \]
the equality holds when and only when \( W_{ij} = W_i W_j' \). Multiplying two sides of (18) by the positive number \( W_i W_j' \) and summing up over \( ij \), one obtains
\[ \sum_{ij} W_{ij} \ln W_{ij} - \sum_i W_i \ln W_i - \sum_j W_j' \ln W_j' \geq 0. \]
This is exactly (17). The lemma is therefore proven.

Suppose \([L] \) is a complete set of commutative dynamical variables of the system, with a complete orthonormal set of eigenstates \(|n\rangle \). The \([L] \) representation of density operator \( \rho \) is a matrix with elements \( \rho_{n,n'} = \langle n|\rho|n'\rangle \). If \( \rho \) itself is included in the set \([L] \), the \([L] \) representation of \( \rho \) is called natural. In a natural representation, the density matrix is diagonal: \( \rho_{n,n'} = W_n \delta_{n,n'} \), in which \( W_n \) is the \( n \)th eigenvalue of \( \rho \), denoting the probability of finding the system being in the state \(|n\rangle \). The information (2) may be written in the form
\[ 1 = \sum_n W_n \ln W_n. \] (19)

One may also consider the information about a specially chosen complete set of commutative dynamical variables \([L] \), with complete set of orthonormal eigenstates \(|m\rangle \). For an ensemble of the systems with the density operator \( \rho \), the probability of finding the system in the state \(|m\rangle \) is
\[ W'_m = \sum_n \langle m|n\rangle W_n \langle n|m \rangle. \] (20)
The definition of the information about the variables \([L] \) is
\[ I[L] \equiv \sum_m W'_m \ln W'_m. \] (21)
Since \(|\langle m|m\rangle|^2 \) are non-negative, and \( \sum_n |\langle m|m\rangle|^2 = \sum_m |\langle m|m\rangle|^2 = 1 \), according to lemma 3 and equation (19) we have
\[ I[L] \leq 1. \] (22)

Now, let us divide the system into two parts \( a \) and \( b \). Suppose \([L_i] \), with \( i = a \) or \( b \), is a complete set of commutative dynamical variables of part \( i \), \(|n_i\rangle \) is their \( n_i \)th eigenstate, and \(|n_i\rangle \) is a complete set of states of part \( i \). Therefore \([|n_a\rangle n_b\rangle] \equiv [|n_a\rangle |n_b\rangle] \) is a complete orthonormal set of states of the system. In the \([L_a L_b] \) representation, The density operator of the system is a matrix, with elements
\[ \rho_{n_an_b,n'_an'_b} \equiv \langle n_a n_b|\rho|n'_a n'_b \rangle. \] (23)
From (20) we see the probability of finding part \( a \) in the state \(|n_a\rangle \) and part \( b \) in the state \(|n_b\rangle \) is
\[ W_{n_an_b} = \sum_n \langle n_an_b|n\rangle W_n \langle n|n_an_b \rangle, \] (24)
with normalization
\[ \sum_{n_a n_b} W_{n_a n_b} = 1. \]  
(25)

The information of dynamical variables \([L_a, L_b]\) is
\[ 1_{L_a, L_b} = \sum_{n_a n_b} W_{n_a n_b} \ln W_{n_a n_b} \leq 1. \]  
(26)

The probability of finding part \(a\) in the state \(|n_a\rangle\) and the probability of finding the part \(b\) in the state \(|n_b\rangle\) are
\[ W_{n_a} = \sum_{n_b} W_{n_a n_b} \quad \text{and} \quad W'_{n_b} = \sum_{n_a} W_{n_a n_b}. \]  
(27)

respectively. In (25-27), it is understood that the summation is over those \(n_a\) and \(n_b\) only, for which \(W_{n_a n_b} > 0\).

The density operator \(\rho_a\) of part \(a\) is reduced from the density operator \(\rho\) of the system. In the representation \([L_a]\), it is a matrix with elements
\[ (\rho_a)_{n_a, n'_a} = \sum_{n_b} \rho_{n_a n_b, n'_a n_b} = \sum_{n_b} \langle n_a n_b | \rho | n'_a n_b \rangle, \]  
(28)

and may be written in a compact form
\[ \rho_a = \text{Tr}_b \rho. \]  
(29)

The subscript \(b\) denotes that the trace is a sum of matrix elements diagonal with respect to quantum numbers of part \(b\) only. Likewise, \(\rho_b = \text{Tr}_a \rho\). Suppose \(\rho_i\) is included in the set \([L_i]\), the probability of finding the part \(i\) in state \(|n_i\rangle\) is its eigenvalue \(W_{n_i}\), and is expressed in (27).

The information about part \(i\) is
\[ i_i = \text{Tr} \rho_i \ln \rho_i = \sum_{n_i} W_{n_i} \ln W_{n_i}. \]  
(30)

From lemma 4 and equations (26,27) we see,
\[ \text{Tr} \rho_a \ln \rho_a + \text{Tr} \rho_b \ln \rho_b \leq \text{Tr} \rho \ln \rho, \]  
(31)

the equality holds when and only when the density operator of the system may be factorized into a direct product of density operators of its parts. We may further subdivide the parts and apply (31) to them again and again, the result is the statement (8). This statement, together with the second law (9) of thermodynamics, is therefore finally proven.

The proof here is quite general. It seems relying on the quantum mechanical effects of state entanglement and its collapse. However, it is still more general. It is an information theoretical proof, relies only on the information conservation (3) and the general relations (27) of the probabilities. The former is a character of dynamics. But it is shared by quantum dynamics and classical dynamics, as well as some dynamics not yet have been discovered at the present
time. The later is purely mathematical. State entanglement and its collapse is only a special way for their realization. They may be realized in classical mechanics or in some unknown mechanics as well. The second law of thermodynamics is therefore almost dynamics independent, except the requirement of information conservation. It may be still exactly true in the future, even though one day people find that the quantum mechanics is only approximate. It is also quite generally applicable, not only to thermodynamics but also to any statistical science, including social science, if the information conservation is true for them. From the proof we learn that the entropy of an isolated system increases only because one loses the correlation information between different parts of the system. It opens a possibility of developing a theory which takes the correlation information into account.