ENTROPY: THE ENIGMA REVISITED

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Abstract: In classical physics entropy of a physical system is proportional to energy no longer available to do physical work. Shannon's work in probability and information theory introduced average information as entropy. Heat equivalent of erasure of one bit of information brought the notion of thermodynamic entropy and information entropy together. Negentropy is used in both information theory and biological processes in living organisms.

Index Terms **–Entropy, Information Entropy, negentropy.**

I. INTRODUCTION

Entropy is a widely used term in various scientific discipline. Historically it was first used by Clausius in 1865.[1] It is central to the second law of thermodynamics which states that in an isolated system any irreversible process increases the entropy. Ludwig Boltzmann and Willard Gibbs introduced entropy in probabilistic set up of statistical mechanics and later it was developed by Max Planck. Von Neumann extended it to quantum mechanics and paved the way for Claude Shannon to use entropy in probability and information theory. The formulation of Maxwell's demon problem initiated the search for physical meaning of information which led Brillouin and Landauer in their quest for it. The concept of entropy has been used in cosmology, biochemistry, life sciences, information theory and even in social sciences also. May be, entropy is the most misused and misunderstood term and often creates confusion about its true meaning and characteristics. There are of course some kind of shared conceptual parallelism between all these concepts but there are differences also. Without understanding these differences, bridging between concepts may create more confusions. In this article the concept of thermodynamic entropy, information entropy and negentropy will be revisited and in the light of the differences among them, the relation of them will be discussed.

II. **Thermodynamic Entropy**

The term entropy was derived from Greek 'en' means 'in' and 'trope' means a turning point.[4] Etymologically it means a form of energy which turns into unavailable energy, i.e. cannot be used to perform work. Clausius, who coined the term 'Entropy', inevitably was inspired by the work of Sadi Carnot. In the mid19th century several investigations were going on about low efficiency of steam engines. Carnot proposed an ideal heat engine which used to work on reversible cycle and extract mechanical work out of engines that ran by virtue of temperature difference between hot reservoir and cold reservoir. That period was particularly an important period for establishing several important concepts in thermodynamics such as 'system', 'surroundings', concept of thermodynamic equilibrium, reversible and irreversible processes, state and path variables etc.[2,3] A thermodynamic system can be classified in categories such as 'isolated', 'closed' and 'open' depending upon the nature of the boundary that is separating it from its surroundings. The state of a system can be specified by means of a set of state variables. So, to characterize a physical system, a set of parameters are required, such as distribution of density, temperature, pressure, velocity, chemical potential etc. Also, thermodynamic states, or, more precisely the change of states, signify thermodynamic processes. Thermodynamic processes can also be categorized in two ways, namely, reversible process and irreversible process. In case of reversible process, the system and its surrounding always are in thermodynamic equilibrium and that can be achieved by quasi static processes where the system is infinitesimally closer to its previous equilibrium state throughout the entire process and the path can be retraced back to its initial state. This is why the name 'reversible' has been derived. The second in the category, i.e. the irreversible process signifies that the retracing of path is not possible and the system is not in equilibrium with its surroundings. All natural processes are irreversible and reversible process, in its perfect sense, does not exist in nature.

There is another way to categorize the thermodynamic processes where the name of the state variable affected during the process is used, namely isothermal, isobaric, isochoric, isentropic, isenthalpic etc.

Getting back to Sadi Carnot's proposed heat engine, one can see that the engine is an idealized one and can only be imagined. Let us suppose an engine is operating between two heat reservoirs, which are at, say, temperatures T_1 and T_2,($T_1 > T_2$) and absorbs heat Q_1 from hot reservoir and rejects heat Q_2 at the cold reservoir in the process. The working substance used in the engine is a perfect gas and operates in four steps, constituting a cycle. All the four steps are reversible. Real life engines are not reversible. So, Carnot proposed that "the best engine operating between a source at T_1 and a sink at T_2, cannot be better in efficiency than Carnot's engine operating between the same temperatures." If efficiency be denoted by η, then $\eta_{real} \leq \eta_{carnot}$.[2, 3]

This set the stage for second law of Thermodynamics. Carnot did not say something explicitly, used caloric theory of heat which eventually came to be erroneous, but his logic was correct. From his derivation it can be written that $\frac{Q_2}{Q_1} = \frac{T_2}{T_1}$ and efficiency of the Carnot's engine as $\eta = 1 - \frac{Q_2}{Q_1} = 1 - \frac{T_2}{T_1}$. It is evident that efficiency can never be equal to one because the heat rejected to the sink Q_2 then must be zero or, the temperature of the sink T_2 must be zero which is unattainable according to third law of Thermodynamics. It can be written that $\frac{Q_1}{T_1} = \frac{Q_2}{T_2} = constant$. Feynman remarked at it that in a reversible process as much ($\frac{Q}{T}$) is absorbed by the sink as is liberated by the source; there is no gain or loss of ($\frac{Q}{T}$).[2] The quantity ($\frac{Q}{T}$) is identified with entropy. An isolated system does not exchange energy or matter with its surroundings. According to first law of Thermodynamics an isolated system can pass only between states of the same global energy. The second law introduces irreversibility, i.e. an isolated system cannot pass from a state of higher entropy to a state of lower entropy. Equivalently it can be said that it is impossible to perform a process whose only final effect is transmission of heat from a cooler to a hotter body. Any such transmission must involve outside work and the overall entropy will rise.

The first and second laws of Thermodynamics together point to the fact that an isolated system will eventually tend to attain the state with maximum entropy among all states having same energy which is the equilibrium state and the reaching of this state is denoted by thermodynamical death of the system. At this state the available energy or the Gibb's free energy becomes zero and the system is left with unavailable energy which cannot be extracted for the performance of work. Entropy is related to unavailable energy. It is from here, the concept of thermodynamic array of time can also be defined.[2]

III. Entropy in Statistical Mechanics

The work of Carnot and Clausius introduced the concept of macroscopic thermodynamical entropy but it was Boltzmann, who gave a deep insight into it. According to him heat is disordered energy. So, in two words the nature of heat is explained. In order to go further it is necessary to talk quantitatively. One must measure heat precisely in terms of numbers. So, to specify heat one must use at least two numbers: one to measure the quantity of energy, the other to measure the quantity of disorder. The quantity of energy is measured in terms of a practical unit called calorie and quantity of disorder is measured in terms of mathematical concept called Entropy.[4]

Though the four laws of thermodynamics formed a robust scaffolding of the macroscopic picture, the inquiry into the microscopic world was going on. In investigating the nature of heat and its relationship with atoms, the statistical interpretation was required. One mole of gas contains roughly 10^{23} number of atoms. Macroscopically the pressure, volume, temperature and entropy describe the properties of it. But to specify completely the behaviour of all its atoms the parameters called degrees of freedom, are required. Specifying the degrees of freedom of 10^{23} number of particles is a formidable task and to simplify, concepts of microstates and probabilities are introduced. In a 6N dimensional space or gamma space all the N(say) particles in the system at a given time can be represented by a single point. The time evolution of the entire system is correspondingly represented by just a trajectory. This trajectory gives the history of evolution of microstates even though the gas is in macroscopic equilibrium.

Let the probability of a microstate j be p_j and ε_j be its energy. Then using Boltzmann distribution

$p_j = \frac{\exp[-{}^{\varepsilon_j}/_{K_B T}]}{\Sigma_j \exp[{}^{-\varepsilon_j}/_{K_B T}]}$, where T is the absolute temperature and K_B is Boltzmann constant.

Gibb's entropy relation is given by $S = -K_B \Sigma_j p_j \ln p_j$. In a macrostate, there exist several microstates of equal energy, volume and number of particles and according to "Equal A-Priori Probability" all the microstates are equally probable. If W is the number of microstates then $p_j = \frac{1}{W}$. So, Gibb's entropy relation gives $S = K_B \ln W$. This is famous Boltzmann equation of entropy which is the epitaph engraved on his tombstone. This equation says that entropy is proportional to the number of microstates available to the system. If the gas particles are colliding with one another, each collision brings about more disorder in the system, leading to a final state of maximum microscopic disorder, a state of maximum entropy which is also the state of thermodynamic equilibrium.[2,3,4]

IV. Information Entropy

Information theory is a field of study concerned with quantifying information for communication. Quantifying the amount of information requires the use of probabilities. So, there is a very close relationship between information theory and probability. The main aim behind quantifying information is the idea of measuring how much surprise is there in an event. Those events which are rare, i.e. the probability of occurrence is low, have high information content and those having high probability of occurrence, have low information content.[5]

Let us suppose in a communication system, m_1, m_2, m_3……etc. are allowable messages with probabilities of occurrences p_1, p_2, p_3…… respectively, so that, $p_1 + p_2 + p_3 + \cdots = 1$. If the transmitter selects messages m_k with probability p_k , by way of definition of the term information, the amount of information conveyed by the system is given by $I_k = log_2 \frac{1}{p_k}$, where I_k is a dimensionless number and conventionally a unit 'bit' is attached to it. If $p_k = \frac{1}{4}$, then $I_k = log_2 4 = 2$ bits. Here the base of the logarithm is taken as 2, for if two possible binary digits or bits may occur with equal likelihood, each with probability 'half', then the correct identification of the binary digits conveys an amount of information $I = log_2 2 = 1$ bit. This is especially useful when binary pulse coded modulation technique is employed. If natural logarithm base is used, the unit is Nat, and for base 10 logarithm unit is 'Hartley'.

If the probabilities of two possible binary digits are not equally likely, one of it conveys more and the other conveys less than one bit of information. If there are M equally likely and independent messages and M=2^N , where Nis an integer, information in each message is $I = log_2 M = log_2 2^N$=N bits.

When two independent messages $m_k \; and \; m_l$ are correctly identified, the amount of information conveyed is the sum of information associated with each of the messages individually. Let $I_k = log_2 \frac{1}{p_k}$ & $I_l = log_2 \frac{1}{p_l}$; messages are independent. The probability of composite message be $p_k p_l$ with corresponding information content of messages m_k & m_l is

$I_{k,l} = log_2 \frac{1}{p_k p_l} = log_2 \frac{1}{p_k} + log_2 \frac{1}{p_l} = I_k + I_l$.

Let there are M independent and different messages m_1, m_2, m_3 ….. with probabilities of occurrence p_1, p_2, p_3 …. . During a long period of transmission, a sequence of L messages has been generated. If L is very large, it is expected that in the L message sequence, $p_1 L$ messages of m_1 , $p_2 L$ messages of m_2 etc. has been transmitted. The total information in such a sequence will be $I_{total} = p_1 L log_2 \frac{1}{p_1} + p_2 L log_2 \frac{1}{p_2} + \ldots$

So, the average information per message interval represented by symbol H, is given by

$H = \frac{I_{total}}{L} = p_1 log_2 \frac{1}{p_1} + p_2 log_2 \frac{1}{p_2} + \cdots = \sum_{k=1}^{M} p_k \, log_2 \frac{1}{p_k}$. This average information is termed as Entropy.

If there is only a single possible message, $p_k = 1$; the receipt of this message conveys no information and if p_k tends to zero, I_k tends to infinity. Since $lim_{p \to 0} \, p \, log \, \frac{1}{p} = 0$ the average information associated with an extremely unlikely message as well as extremely likely message is zero. So, H=0 at p=0& p=1 and maximum value of H occurs at $\frac{dH}{dp} = 0$ which is at p=$\frac{1}{2}$ i.e the two messages are equally likely.[5]

$H_{max} = \frac{1}{2} log_2 2 + \frac{1}{2} log_2 2 = log_2 2 = 1$ bits/message.

If there are M messages, it may be proved that H becomes a maximum when all messages are equally likely. Each message has a probability $p = \frac{1}{M}$ & $H_{max} = \sum \frac{1}{M} log_2 M = log_2 M$. It is clear that the quantity $log_2 \frac{1}{p_k}$ is a measure of unexpectedness of the event k. so the quantity $H = \sum p_k log_2 \frac{1}{p_k}$ or, $H = -\sum p_k log_2 p_k$ is a measure of average unexpectedness of the whole set of outcomes of the experiment.

The information about the state of the system is or should be the information which is available to an outside observer. So, the information must somehow escape from the system and that increased availability of information or the energy contained within the system to perform physical work, must decrease the entropy of the system.

This approach was subjected to many debate and discussions. It made the entropy of a system dependent on the subjectivity of 'knowledge' of an observer.[10,11] The Maxwell's demon problem was based on the assumption that it was possible to acquire information about the parameters of individual particle of a gas contained in a partitioned container, without any expenditure of heat or work. To avoid such paradox, one must agree that acquiring information must increase the entropy of the memory of the observer by a certain amount. Rolf Landauer established that the amount equals to the Boltzmann constant K_B. So, erasing one bit of information from a memory at temperature T results in emission of heat by an amount $K_B T$ to the surroundings. This fact sets limits on the theoretical maximal speed of computers. It also brought the notion of thermodynamical and information entropy together.[8,11]

V. NEGENTROPY

The term negentropy was coined by Erwin Schrödinger in his book 'What Is Life: the physical aspect of the living cell' based on lectures delivered at Trinity College, Dublin in 1943. In it he wrote "what on organism feeds upon is negative entropy".[6] According to Schrödinger, negentropy is entropy with negative sign. In Statistical Thermodynamics entropy is conceptualized as a measure of disorder. In nature, as the processes are irreversible, a system is always be found in the state of maximum disorder. But in the domain of living organisms, the systems are complex and highly organized. A tree from a seed or an animal growing out of an embryo, actually represents a journey towards a more orderly state. So, if δ is the measure of disorder, 1/ δ can be regarded as the measure of order and negentropy can be represented as $\{-S = K_B \frac{1}{\delta}\}$.

As the living system shows a tendency for self-organization thereby decreasing the disorder in it and acquiring information, naturally the entropy should decrease in the process. This fact is in apparent contradiction with the second law. Schrödinger argued that the living organisms are open systems, so they increase the entropy of the surroundings.[6]

But recent studies in biological sciences shows that entropy do increase in the living organisms and in individual cells.[12] In case of biochemical reactions, the term free energy is frequently used. We know $\Delta E = \Delta F + \Delta S$, where F is free energy which is available for work and the energy related to entropy is unavailable. In living cells, most of the reactions occur in adiabatic condition where the entropy is not been generated. Schrödinger admitted this difficulty in discussing the cellular processes. The problem is akin to Maxwell's paradox. In a container having two separate compartments, contains some gas in equilibrium and a demon can open a valve to let the fast-moving molecule in one direction and the slow moving in the other, thereby extracting work from the system. Maxwell's demon was proved to be realized when a solid-state device like diode acts as a rectifier. Similar kind of situation exist in cellular processes where biological membranes are involved and the metabolites are transported from one side to another by way of the function of enzymes. There is no real violation of second law as the rectifiers and biological membranes are non-equilibrium structures which can store energy.[12]

Leon Brillouin in 1949 wrote an article having title "Life, Thermodynamics and Cybernetics" and discussed about information and negative entropy.[7] He inquired into the matter and asked an important question: if information means negative entropy how one can measure the quantity? In 1956, Brillouin in his book 'Science and Information Theory' used the term negentropy for negative entropy and devised a principle named 'negentropy principle of information'. He described the principle as a generalization of Carnot's principle $\Delta(S - I) \geq 0$, where ΔI is the increase in information. Expenditure of negentropy of some other system is necessary to acquire new information. It can be shown that for an isolated system the sum of information and entropy remains constant.[7] The concept of negentropy may be extended to quantum many body systems, in nuclear fusion in solid or liquid metals or in stellar plasmas.[9]

VI. CONCLUSION

Entropy concept was originally introduced by thermal physics as a measure of molecular chaos. Later it was introduced to information theory by Shannon. Von Neumann again extended it to quantum systems by means of density matrix. But the concept has not been limited to Physics and Thermodynamics. The entropy concept has been used to measure uncertainties inherent in stochastic processes , in finance, physiology, neuroscience, ecology and biophysics. But the concept of entropy, as introduced by Clausius, Boltzmann and Shannon remain the main players in the arena. Entropy is a physical, non-negative property and is measurable. So, the concept of negative entropy as introduced by Schrödinger might be wrong. Other disciplines, sometimes distant from Physics and Mathematics, use it rather vaguely and the rigorous quantitative character has not been maintained. It roughly means chaos, decay of diversity or tendency towards uniform distribution.

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