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INFORMATION THEORY AND THERMODYNAMICS I.

C. G. CHAKRABARTI[1], N. G. SARKER[2], CALCUTTA

The paper deals with the study of the statistical characteristics of thermal equilibrium and macrostates of a system from the broader perspective of information theory and statistics.

ТЕОРИЯ ИНФОРМАЦИИ И ТЕРМОДИНАМИКА

В раборе приведены результаты исследований статистических характеристик термического равновесия и макросостояний системы с точки зрения теории информации и статистики.

I. INTRODUCTION

The information theory approach to statistical mechanics developed by Jaynes [1], Ingarden and Urbanik [2] is based on Shannon's measure of entropy or information. In the case of the classical dynamic system the formalism based on Shannon's measure of information gives rise to some difficulties [3], which can be removed by the use of the Kullback discrimination information [4]. In this paper we wish to study the importance of the Kullback information in the statistical theory of thermal equilibrium. The theory developed from the broader perspective of information theory and statistics gives new insight into some basic results and concepts of statistical thermodynamics.

II. SYSTEM AND STATE-SPACE

Let us consider a classical dynamic system. The microstate of the system are the phase points on the phase space Γ. The statistical structure of the microstates is given by the σ-algebra $\mathscr{A}$ of the set of microstates and the probability density $\varphi(\omega)$ of microstates defined on Γ. Let $X(\omega)$ be the energy (Hamiltonian) of the system

[1] Department of Applied Mathematics University of Calcutta, 92, Acharya Prafulla Chandra Road, CALCUTTA – 700009, India.

[2] S. N. Bose Institute of Physical Sciences University of Calcutta, 92, Acharya Prafulla Chandra Road, CALCUTTA – 700009, India.

and is the only macrovariable necessary to be describe the system. Let $\mathscr{A}_x$ be the sub-algebra induced by $X(\omega)$. The probability density of $X(\omega)$ is given by the *"coarse-grained"* probability [4]

$$f(x)=E_m(\varphi(\omega)|X(\omega)=x)=\int \varphi(\omega)\delta(X(\omega)-x)\,\mathrm{d}m(\omega), \tag{1}$$

where the integration is with respect to the Liouville measure (volume) m of the phase-space Γ. The energy $X(\omega)$ transforms the space of microstates into that of X-space, the subsets of which represent the macrostates of the system. The sub-algebra $\mathscr{A}_x$ and the probability distribution of $X(\omega)$ determine the statistical structure of the macrostates of the system.

III. MACROSTATES AND DISCRIMINATION INFORMATION

Fundamental to statistical mechanics is to understand the macrostates of the system. The different macrostates (or thermodynamic states) of the system are characterized by the averages of $X(\omega)$ and can be parametrized by a parameter β. Let φ_β be the probability density of microstates corresponding to the macrostate represented by the parameter β. Then the measure of directed divergence between the macrostates corresponding to the parametric values β and β_0 is given by the Kullback discrimination information [4]

$$I(\varphi_\beta)|\varphi_{\beta_0})=\int \varphi_\beta(\omega)\log\frac{\varphi_\beta(\omega)}{\varphi_{\beta_0}(\omega)}\,\mathrm{d}m(\omega). \tag{2}$$

The quantity $I(\varphi_\beta|\varphi_{\beta_0})$, according to Rényi [5], is the gain of information about the system at the macrostate β over that of the macrostate β_0. The corresponding discrimination information for the *"coarse grained"* distribution of $X(\omega)$ is given by

$$I(f_\beta|f_{\beta_0}) = \int f_\beta(x)\log\frac{f_\beta(x)}{f_{\beta_0}(x)}\,\mathrm{d}x. \tag{3}$$

There is in general a loss of information for the *"coarse-graining"* of microstates and this corresponds to the discarding of the available information which is irrelevant or nearly so for the particular prediction desired [1b]. For the system described by the energy $X(\omega)$ only, this results in the assumption of the equality [6]

$$I(\varphi_\beta|\varphi_{\beta_0})=I(f_\beta|f_{\beta_0}). \tag{4}$$

Mathematically, the equality (4) holds if and only if [4]

$$\frac{\varphi_\beta(\omega)}{E_m(\varphi_\beta(\omega)|X(\omega)=x)}=\frac{\varphi_{\beta_0}(\omega)}{E_m(\varphi_{\beta_0}(\omega)|X(\omega)=x)}. \tag{5}$$

The equality (5) has an important physical significance. It states that the probability

of finding a system in one of the available macrostates will be equal, being consistent with the principle of equal weight [7]. In fact, for the canonical states φ_β and φ_{β_0}, as we shall see later on, the equality (5) for all values of the parameter β implies the thermodynamic necessity of the invariance of the structure function of statistical weight [8].

IV. MACROSTATES: PROBABILITY AND FLUCTUATION

Let us now suppose that the probability distribution $f_{\beta_0}(x)$ corresponds to the complete (or total) equilibrium of the system with the environment (or heat-reservoir) and $f_\beta(x)$ to that of a frozen equilibrium state. Then the discrimination information $I(f_\beta|f(_{\beta_0})$ is the gain of information of the frozen equilibrium state over that of the complete equilibrium. The probability density $f_{\beta_0}(x)$ for the complete equilibrium can be determined by minimizing the discrimination information $I(f_\beta|f_{\beta_0})$ subject to the constraint $\bar{X}=\bar{X}(\beta_0)$ characterizing the complete equilibrium of the system with the environment. The minimization consists in the discarding of all additional or surplus information of the frozen equilibrium state over that of the complete equilibrium. Let at any stage $\beta=\beta_0+\Delta\beta_0$, where the deviation $(\Delta\beta_0)$ is either due to spontaneous fluctuation in equilibrium or due to the relaxation process. For small $(\Delta\beta_0)$, we have [4]

$$I(f_{\beta_0+\Delta\beta_0}|f_{\beta_0})=\frac{1}{2}H_x(\beta_0)(\Delta\beta_0)^2, \tag{6}$$

where

$$H_x(\beta_0)=\int\left[\frac{\delta}{\delta\beta_0}\log f_{\beta_0}(x)\right]^2 f_{\beta_0}(x)\,\mathrm{d}x \tag{7}$$

is the Fisher information giving a measure of the sensitivity of $X(\omega)$ to a small change in the parameter β_0. The probability density $f_{\beta_0}(x)$ determined by minimizing (6) subject to the constrain $\bar{X}=\bar{X}(\beta_0)$ is given by the canonical distribution [6]

$$f_{\beta_0}(x)=\exp\{\lambda(\beta_0)x\}\,h(x)/Z(\lambda(\beta_0)), \tag{8}$$

where the function $h(x)$ is independent of β_0 and is the structure function or statistical weight. The function $\lambda(\beta_0)$, determined by the second law of thermodynamics, is the universal function $X(\beta_0)=-1/kT_0$, k being Boltzmann's constant, T_0 the absolute temperature. Without loss of generality we take $\lambda(\beta_0)=-\beta_0$ so that β_0 is the natural temperature $1/kT_0$.

Let us now consider the probability of fluctuation (or deviation)$f_{\beta_0|\beta}(x)$ from the canonical state f_{β_0} to the canonical state f_β. The discrimination information $I(f_\beta|f_{\beta_0})$ measures the gain of information associated with the event of fluctuation from the state f_{β_0} to the state f_β. Again the information associated with the same event of fluctuation is given by the self information $-\log f_{\beta_0|\beta}(x)$. So the probability of fluctuation is given by

$$f_{\beta_0|\beta}(x) \sim e^{-I(f_\beta|f_{\beta_0})}. \tag{9}$$

For canonical distribution we have [9]

$$kI(f_\beta|f_{\beta_0}) = \{S(\beta_0) - S(\beta)\} - \frac{1}{T_0}\{\bar{X}(\beta_0) - \bar{X}(\beta)\}, \tag{10}$$

where $S(\beta)$ is the entropy (thermodynamic) of the system at the frozen equilibrium state and $S(\beta_0)$ is that for the system at complete equilibrium. So the probability of fluctuation for a small deviation of macrostate can be written as

$$\bar{\omega} \sim e^{-\beta_0 \Delta F_0}, \tag{11}$$

where

$$F_0 = \bar{X}(\beta_0) - T_0 S(\beta_0) \tag{12}$$

is the free energy of the system.

V. MACROSTATES AND CRITERIA OF SUFFICIENCY

Let us now study the importance of sufficiency – a reduction principle of statistics, in the statistical interpretation of macrostates and thermal equilibrium of the system. If in statistics the equality (4) holds for all values of the parameter β (including the value β_0), then the energy $X(\omega)$ is called a sufficient statistic and $\mathscr{A}_x$ a sufficient sub-algebra for the family of probability densities $\{\varphi_\beta\}$ [4].

The macroscopic description is thus equivalent to the sufficient partitioning of the microstates into equivalent classes of macrostates for which there is no loss of the discrimination $I(\varphi_\beta|\varphi_{\beta_0})$. Thermodynamically, this equivalent to the reversible change or transformation of the system through the different macrostates (or thermodynamic states) represented by the values of the parameter β.

The energy $X(\omega)$ which is sufficient for the macroscopic description, is minimal (or least) sufficient for the minimization of (6) leading to the canonical distribution (8). This leads to the important criteria of sufficiency due to Mandelbrot according to which the energy of a closed system in thermal equilibrium of a heat-reservoir is minimal sufficient for the determination of the temperature of the heat reservoit [10]. The thermal (complete) equilibrium of a system is thus equivalent to the minimal sufficiency of the energy $X(\omega)$ of the system and this, consistent with the *"coarse grained"* interpretation of thermal equilibrium, corresponds to the maximum reduction of *"coarse graining"* of the microstate subject to the given constraints [11].

Let us consider an important application of these criteria. From the minimization of (6) it follows that the spread $\Delta^* X$ of $X(\omega)$ in thermal equilibrium is given by the lower-bound of the root mean-square deviation of $X(\omega)$, that is [6]

$$\Delta^* X = [\text{Min}\ (\overline{\Delta X})^2]^{1/2}. \tag{13}$$

If δX be the width of variation of $X(\omega)$, then for minimal sufficient $X(\omega)$, we have $\Delta^* X \simeq \delta X$ [12]. This leads to the important result that the canonical distribution (8) is valid over a range of width δX, which is of the same order of magnitude as the spread $\Delta^* X$ [13]. The condition $\Delta^* X \simeq \delta X$ is a characteristic of the macrostate corresponding to the complete equilibrium of the system. Under this condition the entropy (thermodynamic) of the system

$$S(\beta_0) = k[\beta_0 \bar{X}(\beta_0) + \log Z(\beta_0)] \tag{14}$$

reduces to the Boltzmann form [14]

$$S(\beta_0) = k \log h(\bar{X}(\beta_0)), \tag{15}$$

which shows that in the thermodynamic limit of a large number of degrees of freedom of a macroscopic or thermodynamic system both the canonical and microcanonical entropies become identical [15].

VI. CONCLUSION

The paper which is a modification of an earlier work [6b] attempts to study the importance of the Kullback information in statistical thermodynamics. The sufficiency – a reduction principle of statistics, gives a general statistical characterization of macrostates and thermal equilibrium. The theory developed from the broader perspective of information theory and statistics attempts to give a new approach and insight to some basic problem of statistical thermodynamics and helps to study the close interrelations between thermodynamics and statistics.

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