GLOBAL JOURNAL OF PURE AND APPLIED SCIENCES VOL. 8, NO. 1, JANUARY 2002:143-148

THE ENTROPIC FORMULATION OF STATISTICAL MECHANICS USING THE ISING MODEL.

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(Received 19 April 2001 ; Revision accepted 15 June, 2001)

ABSTRACT

The computation of the partition function. Z_n of a system is of paramount importance in Statistical Mechanics. as Z_n. gives every other thermodynamical information of the system. This method can be tedious because of the complicated expressions of the partition function especially in 2 or 3-dimensions which demands rigorous mathematical analysis like series expansion. This paper gives an "alternative method" of formulating Statistical Mechanics using Ising model to give the entropy of the system directly: the entropy being in fact. the more important fundamental variable than the free energy. F. in thermodynamics.

Keywords: Partition function. entropy. configuration. fundamental constraint. energy.

1. INTRODUCTION

In statistical analysis of an equilibrium thermodynamic system. Gibb's famous prescription is to determine the partition function. Z_N of the system. from which follows all the thermodynamically relevant information. That is we need

$$Z_n = (N!h^{gN})^{-1} \iint exp.\ (-\beta H)\ dp\ dq.\ (classical)$$

$$Z_n = Trace\ [exp.\ (-\beta H).\ (quantum) \qquad (1)$$

where $H = H_N(p.\ q)$ is the Hamiltonian function (classical) or operator (quantum) of the system of N particles in g-dimensional physical space in thermal equilibrium with a heat reservoir of temperature. T. defined by $\beta = 1/kT$ and h is Planck's constant: (Feynman 1972. Kittel 1985). The generalised momentum of each particle is $p_i \in R^g$ $i = 1, 2, \ldots N$: and the generalised position q of each particle is confined to $\Lambda \subset R_g$. called the "box" of physical volume V. so that $p = (p_1, p_2, \ldots, p_{Ng}) \in R^{Ng}$ and $q = (q_1, q_2, \ldots q_{Ng}) \in \Lambda^N \subset R^{Ng}$. In the limit $N \to \infty$. N/V *finite*, we obtain from Z_N the free energy. $F = F(\beta, V, N)$ as $F = -kTlnZ_N$ and the internal energy $U = \partial lnZ_N / \partial\beta$. From F. we obtain S. entropy. $S = S(U, V, N)$ either by using the thermodynamic relation: $S = (U - F)/T$, or equivalently. $S = -k\Sigma\rho ln\rho$ with $\rho = exp.(-\beta H)/Z_N$ or from the Legendre transform.

$$F(\beta, V, N) \to S(U, V, N) = \frac{\beta\partial\bar{F}}{\partial\beta} - F.\ \bar{F} = \beta F. \qquad (2)$$

in which $\bar{F}$ is the Massieu function of S. each method involving the knowledge of Z_N (or equivalently of F).

1.1 ENTROPIC FORMULATION

In the postulatory formulation of thermodynamics. which (Wightman 1979) has appropriately called neo-Gibbsian thermodynamics. perhaps best exemplified by *Callen* (Callen 1980). $S(U, V, N)$ is considered as the fundamental relation: (Akin-ojo 1958).

In his paper. (Akin-Ojo 1988). had put up the following arguments:-

(a) that although Z gives F and therefore S. $F(\beta, V, N)$ is a "derived" thermodynamics potential. Whereas. given that statistical mechanics is the foundation of thermodynamics. we should be able to obtain the fundamental relation $S = S(U, V, N)$ of the thermodynamics directly from statistical mechanics of an open system (open with respect to energy or some important attribute).

(b) Suppose we are satisfied with the indirect route of obtaining S from $F = -kTlnZ_N$: then for the case of the system with a homogeneous first-degree Lagrangian. $L = L(q, \dot{q})$ in $\dot{q} = v$: i.e.

$$L(\lambda v, q) = \lambda L(v, q),\ \lambda \in \Re_+ \qquad (3)$$

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the so called partition function is not defined from *(1)*. This is because by Euler's theorem, the Hamiltonian $H(p,q) = v\partial L/\partial v - L$ is identically zero under such condition.

For such reasons, we resort to this alternative method referred to as the "entropic formulation" of statistical mechanics: (Ituen 1989). The later method involves replacement of partition function with the volume of the phase space G given by

$$G = (N!h^{gN})^{-1} \iint C \times D \, dp \, dq. \qquad (4)$$

with the definition $G = \{p:f(p,q) \le \gamma\}$, $q \in D \subset \Re^{Ng}$ and γ is a quantity proportional to the expectation value of some important attribute or some constant of motion $f(p,q)$ such as the internal energy $U = \langle H(p,q) \rangle$. We emphasise that f(p,q) or U is not necessarily the total energy of the system, but part specified by the n degree of freedom. Physically C x D gives the region in phase space allowed the system. The existence of C as a nonempty, bounded, convex set [or equivalently, of f(p,q)] constitutes what we call a fundamental constraint on the system. Using Boltzmann's prescription, we get the fundamental relation (Shannon 1948). $S = S(\gamma,V,N) = k\ln G$, $G = G(\gamma,V,N)$. At quantum level $G = \Gamma$, the number of configurations or microstates consistent with a macrostate specified by the fundamental constraint. Then by Planck/Boltzmann's relation we can have entropy as

$$S = S(U,V,N) = k\ln\Gamma \qquad (5)$$

This relation displays more clearly how the available energy is shared among the energy levels.

In this paper, we calculate the two types of entropies namely S_G (from Gibb's prescription) and S_B (from Boltzmann's prescription) using Ising model in a bid to compare the two methods, viz "partition function" method and entropic formulation method. In addition, we try to answer the question: How large must N be practically to satisfy the thermodynamic limit $N \to \infty$?

2. ISING MODEL

Ising model is a crude similitude of the structure of a physical ferromagnetic substance as containing a domain. As stated in Ituen's work: (Ituen 1989), it is a dichotomic system of +1 or -1, on or off, up or down, present or absent, etc., invented by E. Ising. Its equivalence are lattice gas and binary alloy.

In the Ising model of ferromagnet, the system is considered as an array of N fixed points called lattice sites that form an n-dimensional periodic lattice (n = 1,2,3). The geometrical structure of the lattice may be cubic or hexagonal. Associated with each lattice site is a spin variable $\mu = (1,2,3\ldots,N)$ which is a number that is either +1 or -1. There are no other variables. If $\mu = +1$, then the i-th site is said to have spin up, but if $\mu = -1$, it is said to have spin down. A given set of numbers $\{\mu_i\}$ specifies a configuration of the whole system. The Hamiltonian of the system in the configuration specified by $\{\mu_i\}$ is defined to be

$$H\{\mu_i\} = -\sum_{(ij)} \varepsilon_{ij}\,\mu_i\mu_j - B\sum_{i=1}\mu_i \qquad (6)$$

where the symbol *(ij)* denotes a nearest neighbour pair of spins. There is no distinction between *(ji)* and (ij). Thus, sum over (ij) contains $\gamma N/2$ terms where γ is the number of the nearest neighbour of any given site.

The interaction energy ε_{ij} and the external magnetic field, B, are given constants. For simplicity, we specialise the model to the case of isotropic interactions, so that all are equal to a given number J. Thus the Hamiltonian will be taken as:

$$H\{\mu_i\} = -J\sum_{(ij)}\mu_i\,\mu_j - B\sum_{i=1}^{N}\mu_i \qquad (7)$$

The case J>O corresponds to ferromagnetism while the case J<Q corresponds to antiferromagnetism. Equation (7) is for the one-dimensional model and can be re-written as:

$$H\{\mu_i\} = -J\sum_{(ij)}\mu_i\mu_{j-1} - B\sum_{i=1}^{N}\mu_i$$

For two dimensional, we have (Ituen 1989).

$$H\{\mu_i\} = -J\left(\sum_{i=1}^{m-1}\sum_{j=1}^{m}\mu_i\mu_{j+1j} + \sum_{i-1}^{m}\sum_{j=1}^{m-1}\mu_i\mu_{j+1} - B\sum_{i=1}^{m}\sum_{j=1}^{m}\mu_{ij}\right) \qquad (8)$$

3. RESULTS AND DISCUSSION

We start by computing the number of configuration. F. consistent with the fundamental constraint $f \leq \gamma$ where f is the expectation value of H. neglecting the term with B, the magnetic field strength and γ is the available energy. The quantity g is the actual available energy in the system. So $\Gamma = \Gamma(\gamma N)$. With a particular value of N, we obtain S_B for different values of Γ depending on the values of γ, the available energy.

Figure 1 shows the case for N = 16 in one dimension

Table 1: Boltzmann's entropy for N = 16

γ (J)	Γ	$\frac{S_B}{k} = \ln \Gamma$
1	45638	10.729
3	55648	10.927
5	61654	11.029
7	64384	11.072

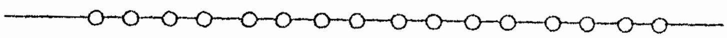

Figure 1: 16 spin arranged in one dimension

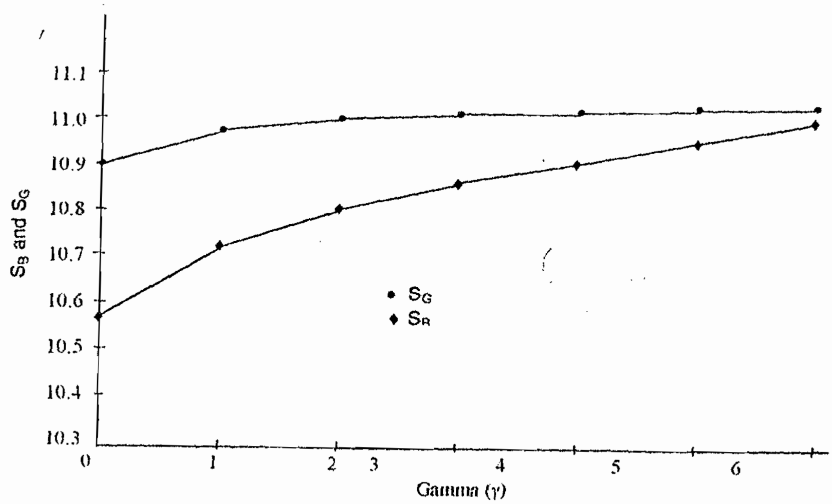

Figure 2: S_B and S_G vs Gamma

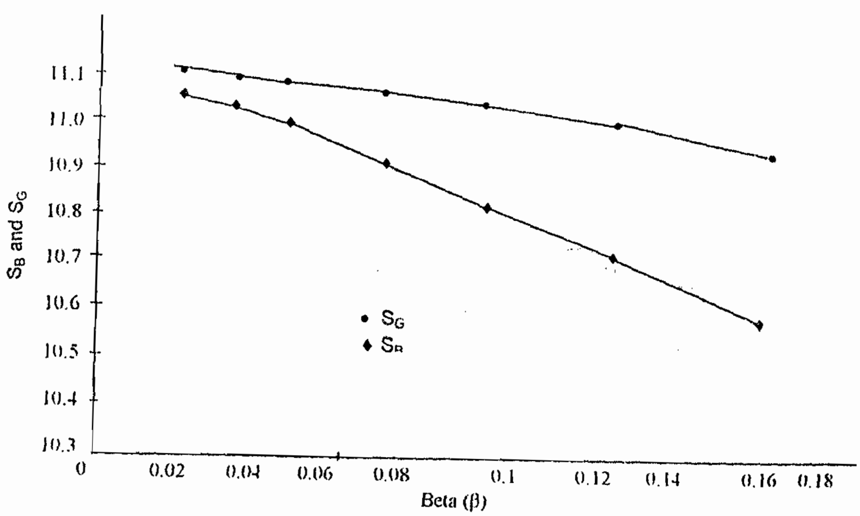

Figure 3: S_B and S_G vs Beta

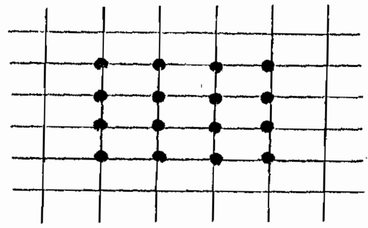

Figure 4: 16 spins arranged in 2-dimensions

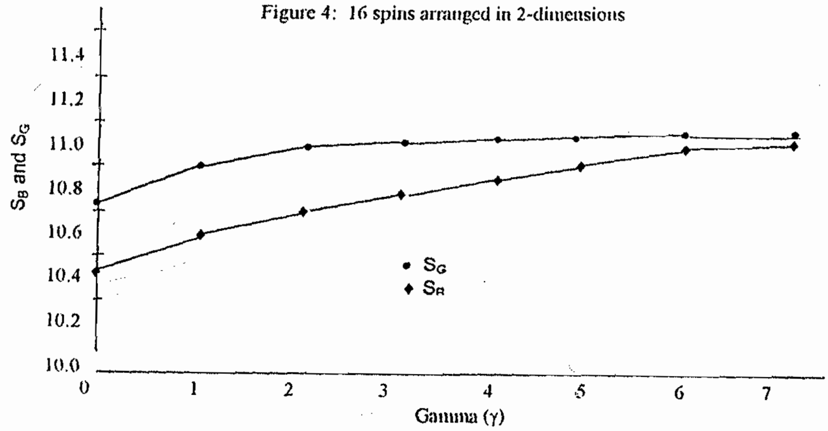

Figure 5: S_B and S_G vs Gamma

By Lagrange interpolation:

$$S = \frac{(\gamma-\gamma_2)(\gamma-\gamma_3)(\gamma-\gamma_4)}{(\gamma_1-\gamma_2)(\gamma_1-\gamma_3)(\gamma_1-\gamma_4)} \times S_1 + \cdots \frac{(\gamma-\gamma_1)(\gamma-\gamma_2)(\gamma-\gamma_3)}{(\gamma_4-\gamma_1)(\gamma_4-\gamma_2)(\gamma_4-\gamma_3)} \times S_4 \quad (9)$$

(Press et al)

$$S_B/k = 0.0008g^3 - 0.019g^2 + 0.165g + 10.58 \quad (10)$$

$$\frac{\delta S_B}{k\delta\gamma} = \beta = 0.0024\gamma^2 - 0.038\gamma + 0.165 \quad (11)$$

Table 2: Comparing S_B and S_G for N = 16

γ (J)	$\frac{S_B}{k}$	β	$U = \frac{\delta \ln Z_{16}}{\delta\beta}$	$F = \frac{-1 \ln Z_{16}}{\beta}$	$\frac{SG}{k} = \beta(U - F)$
0	10.58	0.165	-2.45	-64.45	10.89
1	10.73	0.128	-1.92	-86.94	10.97
2	10.84	0.099	-1.48	-112.77	11.02
3	10.93	0.073	-1.09	-152.47	11.05
4	10.99	0.051	-0.77	-217.84	11.07
5	11.03	0.035	-0.53	-317.12	11.08
6	11.06	0.023	-0.35	-482.36	11.09

(See Figures 2 & 3).

Figure 4 shows the case for N = 4 x 4 = 16 in 2 dimensions.

Table 3: Boltzmann's entropy for N = 16 in two dimensions.

γ (J)	Γ	$\frac{S_B}{k} = \ln \Gamma$
1	38504	10.559
3	48488	10.789
5	55832	10.930
7	60760	11.015

By Lagrange interpolation.

$$S_B/k = 0.0007\gamma^3 - 0.017\gamma^2 + 0.175\gamma + 10.40 \quad (12)$$

$$\frac{\delta S_B}{k\delta\gamma} = \beta = 0.0021\gamma^2 - 0.034\gamma + 0.175 \quad (13)$$

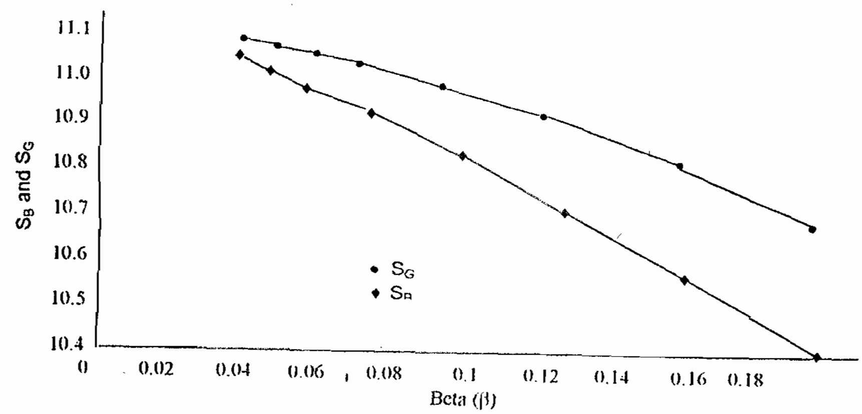

Figure 6: S_B and S_G vs Beta

Table 4: Comparing S_B and S_G for N = 16 in two dimensions.

γ (J)	$\frac{S_\beta}{k}$	β	$U = \frac{\delta \ln Z_{16}}{\delta\beta}$	$F = \frac{-1\ln Z_{16}}{\beta}$	$\frac{S_G}{k} = \beta(U - F)$
0	10.40	0.175	-4.35	-65.51	10.70
1	10.56	0.143	-3.52	-79.29	10.84
2	10.69	0.115	-2.80	-97.83	10.93
3	10.79	0.092	-2.23	-121.66	10.99
4	10.87	0.073	-1.76	-152.80	11.03
5	10.94	0.058	-1.40	-191.91	11.05
6	10.99	0.047	-1.13	-236.53	11.06
7	11.03	0.040	-0.96	-277.73	11.07

(See Figures 5 & 6)

4. CONCLUSION

(a) Generally, the difference $\Delta S = S_G - S_B$ approaches zero as energy, g, becomes large or when $\beta = 1/kT$ is small i. e. when temperature is high. Besides $\Delta S > 0$, which is in agreement with (Jaynes, 1965).

(b) That the two curves for S_G and S_B are similar in each case, and the observation is consistent for both 1 and 2 dimensional, is a confirmation that entropic formulation method (which yields S_B) can reliably replace the "STANDARD" method (which yields S_G) especially at high temperatures or high energies.

(c) The similarity in S_G and S_B which appears more conspicuous in the 2-dimensional than 1-dimensional model is as expected because for the same N, the former has a larger number of degrees of freedom than the later.

(d) The results so obtained for N=16 are quite reasonable for both dimensions. As such, we can deduce from this work that N=16 is large enough to practically satisfy the thermodynamic limit, $N \rightarrow \infty$. That is, the infinity of the thermodynamic limit is not too far.

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