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On the time evolution of the Boltzmann entropy

By

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1. Introduction.

Among the fundamental problems of statistical mechanics one of the utmost interest is the justification of the second law of thermodynamics, or the explanation of the apparent conflict between the microscopic dynamical reversibility and the macroscopic irreversibility. The following things are well known; 1) the entropy (fine-grained entropy) does not change with time and the values of dynamical variables invariant with respect to the time reversal transformation ($t \to -t$, $p \to -p$) can not increase monotonically for all initial conditions because of the reversibility of mechanics, and 2) any continuous dynamical variable can not evolve monotonically all along the time because of Poincarè's recurrence theorem. Several ways to avoid these difficulties are to take the definitions of entropy based not on the fine-grained description provided by an ensemble density, which satisfies Liouville's equation, but on the coarse-grained [1] [2] [3] [4] or reduced description associated with a kinetic equation such as Boltzmann's equation [5] [6] or the master equation [7]. These definitions depend on the averaging of the ensemble density on the phase-space cell in the case of the coarse-grained description and on the assumption under which the kinetic equation holds or on the introduction of Markov process in the case of the reduced description. A quite different definition is proposed by Prigogine [8] and Misra [9]. In their definition the entropy does not appear to have the additive property [10].

For the isolated finite dynamical system it is impossible, as already we noted, to define rigorously a nonequilibrium entropy as a dynamical variable if we require that the increasing law of the entropy should be strictly realized. But these circumstance will not deny the possibility to be able to prove the increasing law of the entropy rigorously in the following sense; there exists some increasing function $f(t)$ and some small $\varepsilon > 0$ for almost nonequilibrium initial states ω such that the inequality $|S(T_t\omega) - f(t)| < \varepsilon$ holds for a very long time interval, where $T_t\omega$ represents the time evolutuin of ω. Of course it is an extremely difficult problem to prove this statement exactly.

In this paper we prove the above statement in a somewhat weakened form, namely we introduce the "Boltzmann entropy $S(\omega)$", which will be defined, and prove the inequality $S(T_t\omega) \geqq S(\omega) - \varepsilon$ for almost ω and a very long time interval. This

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statement is compatible with the reversibility and Poincaré's recurrence theorem.

The definition of the entropy bases on counting the Komplexion of microscopic states under the partition of μ-space (one particle phase space); that is, for a partition of the μ-space $\mathscr{P}$: $\mu=\mu^1 \cup \mu^2 \cup \cdots \cup \mu^\rho$ the Boltzmann entropy $S_{\mathscr{P}}(\omega)=S(\omega)$ is defined by

$$S(\omega)=-\sum_{j=1}^{\rho}\frac{n_j(\omega)}{n}\log\frac{n_j(\omega)}{n},$$

where n is the number of particles of the system and $n_j(\omega)$ is the number of particles which are in the cell μ^j under the microscopic state ω [11] [12]. In connection with Boltzmann's H-theorem Ehrenfest [2] [13], Kac [14], ter Haar et al [15], and Klein [16] studied this entropy. In their studies the time evolution was given by Markov process. Hereafter we consider a simple but basic partition $\mathscr{P}_0$ defined by the sings of momentums of particles (its exact definition is given later).

We note here that in our dynamical study for a time dependence of this entropy we need not assume dynamical properties such as ergodicity, mixing or K-property [17] nor probabilistic postulates. Furthermore we emphasize that our argument is based only on taking the number of particles into account, whose significance is well known [18] [19], and on the geometrical properties of the energy surface and the vector field induced by Hamilton flow. Recently Misra et al [20], Courbage et al [21], Goldstein [22], and Goldstein and Penrose [4] show that ergodic properties such as mixing or K-property are relevant to the problems of nonequilibrium statistical mechanics. These ergodic propertiesis, however, the concept unrelated to the size of the number of particles that is a premise in statistical mechanics. Moreover it is very difficult to show these properties for real systems. Therefore it will be meaningful to show that without requiring such dynamical properties the geometrical properties, for which we take the size of the number of particles into account, play an important role for the investigation of the increasing law of the entropy.

Our result is the following; under a certain weak condition on the interaction potential (we call this the condition for the kinetic activity) the entropy $S(T_t\omega)$ defined by the simple partition $\mathscr{P}_0$ does not decrease from the intial nonequilibrium value for a time interval $|t|\leqq e^{\beta n}$ except for an extremely small set of initial states of order of $e^{-\alpha n}$, where ω is a phase point, $T_t\omega$ is the solution of Hamilton equation with the initial condition ω, n is the number of particles ($\sim 10^{23}$) and α, β are positive constants independent of n. We note here again that this result is compatible with the reversibility and does not contradict Poincaré's recurrence theorem because, though the time interval$(-T, T)$, $T=e^{\beta n}$, is extremely long, it is short compared with the recurrence time.

Our main idea is to concentrate our attention on each "entropy band $\Omega_{[S_b,S_a)}$" (defined later) on the energy surface specified by the entropy values. We will see that when the number of particles is large enough the structure of these entropy bands has a remarkable geometrical properties, i) the volume of the entropy band is extremely large compared with the area of its "lower boundary" which abuts the lower entropy band and ii) the entropy band with the equilibrium entropy value occupies a greater part of the energy surface. This structure of the entropy bands suggests strongly that the entropy has a tendency toward increasing in time, although our statement asserts only that the entropy is non-decreasing in time.

Now let us formulate our problem more precisely.

2. Main result.

We consider a system composed of $N=2n$ particles in a finite box V in the f-dimensional space $\boldsymbol{R}^f$ interacting each other. The Hamiltonian of this system is given by

$$H(p,q)=\sum_{i=1}^{N}\frac{1}{2m}p_i^2+U(q_1,\dots,q_N)$$

where $p_i=(p_i^1,\dots,p_i^f)\in\boldsymbol{R}^f$ and $q_i=(q_i^1,\dots,q_i^f)\in V$ are momentum and position of the i-th particle.

We assume that the potential $U(q_1,\dots,q_N)$ is a smooth function with the range $\{\boldsymbol{R}\cup\infty\}$, and when some particle approaches to the boundary ∂V of the box V, $U(q_1,\dots,q_N)$ increases to infinity. We denote a phase point $(p,q)=(p_1,\dots,p_N,q_1,\dots,q_N)\in R^{fN}\times V^N$ by ω.

Let

$$\mathscr{P}_0:\ \mu=\mu_+\cup\mu_-=\boldsymbol{R}^f\times V$$

where $\mu_\pm=R^f_\pm\times V$, $R^f_+=\{p^1,\dots,p^f)\in R^f;\ p^1\geqslant 0\}$, $R^f_-=R^f-R^f_+$, be a partition of the μ-space (one particle phase space). By means of the partition $\mathscr{P}_0$ of the μ-space, we define the Boltzmann's entropy $S(\omega)$ as follows

Definition 1.

$$S(\omega)=-\frac{n_+(\omega)}{N}\log\frac{n_+(\omega)}{N}-\frac{n_-(\omega)}{N}\log\frac{n_-(\omega)}{N}$$

where $n_\pm(\omega)=\#\{i;\ (p_i,q_i)\in\mu_\pm\}$.

We denote the range of $S(\omega)$ by $\mathscr{R}_n(S)$ for some large n. Let S_{eq} be the maximum value of the entropy under the condition $H(p,q)=E$ where E is some total energy. Clearly $0\leqq S(\omega)\leqq S_{eq}$. Before we state our result let us make some definitions. The energy surface is defined by

Definition 2.

$$\Omega_E=\{\omega\in\boldsymbol{R}^{2fn}\times V^{2n};\ H(p,q)=E\}$$

The entropy band, a subspace of Ω_E specified by an interval of the entropy values, is defined by

Definition 3.

$$\Omega_{[S_b,S_a)}=\{\omega\in\Omega_E;\ S_b\leqslant S(\omega)<S_a\},\ S_b,\ S_a\in\mathscr{R}_n(S).$$

We denote the boundary of a region G by ∂G. We define the upper and lower boundary of the entropy band $\partial^{(+)}\Omega_{[S_b,S_a)}$, $\partial^{(-)}\Omega_{[S_b,S_a)}$, respectively, by

Definition 4.

$$\partial^{(+)}\Omega_{[S_b,S_a)} = \partial\Omega_{[S_b,S_a)} \cap \partial\Omega_{[S_a S_c)}$$

$$\partial^{(-)}\Omega_{[S_b,S_a)} = \partial\Omega_{[S_b,S_a)} \cap \partial\Omega_{[S_d,S_b)}$$

for $S_d < S_b < S_a < S_c$ in $\mathscr{R}_n(S)$.
Let $\{T_t\}$ be the time evolution maps, namely $T_t\omega_0 = \omega(t;\, \omega_0) \in \boldsymbol{R}^{2fn} \times V^{2n}$ is the solution of the Hamiltonian equation with the initial condition ω_0.

Now our assertion is the following:

Theorem. *We assume that for some positive constants* λ_1, λ_2,

$$\text{(A1)} \qquad \sum_{i=1}^{2n} \left[\left(\frac{d}{dt} p_i \right)^2 + \left(\frac{d}{dt} q_i \right)^2 \right] < n^{\lambda_1} \quad \text{on } \Omega_E,$$

$$\text{(A2)} \qquad \frac{1}{\kappa(E;\, H)} \equiv \frac{\int_{q\in D} dq[2m(E-U)]^{fn-\frac{3}{2}}}{\int_{q\in D} dq[2m(E-U)]^{fn-1}} < n^{\lambda_2}$$

for large n,
where

$$D = \{q \in V^{2n};\, E - U(q) \geqslant 0\}\,.$$

Then for any pair S_a, S_b, *with* $0 \leqq S_b < S_a \leqq S_{eq}$ *in* $\mathscr{R}_n(S)$ *there exist positive constants* $\alpha = \alpha(S_b, S_a)$, $\beta = \beta(S_b, S_a)$ *and* $k = k(S_b, S_a)$ *independent of n such that*

$$\frac{|\{\omega \in \Omega_{[S_b,S_a)};\, S(T_t\omega) \geqq S_b \text{ for } |t| < e^{\beta n}\}|}{|\Omega_{[S_b,S_a)}|} > 1 - ke^{-\alpha n}$$

where $|\cdot|$ *denote the volume of a region measured by the Liouville measure on the energy surface. (The constnts* α, β, k *will be given in the proof explicitely.)*

We remark that the condition (A1) is satisfied for the many models. As for condition (A2) we will give an example, which satisfies this one, in section 4; we shall call $\kappa(E;\, H)$ the index of kinetic activity.

This theorem depends only on the following two geometrical lemmas.

Lemma 1. *Let* $(M, \psi_t, d\lambda)$ *be a smooth dynamical flow* ψ_t *on a manifold* M *with a* ψ_t*-invariant smooth measure* $d\lambda$ *and a metric* $|||\cdot|||$, *and* Γ *be a piece-wise smooth hypersurface in* M. *Then*

$$|\bigcup_{|t|\leqq T} \psi_t \Gamma| \leqq 2T|\Gamma|\ \|\dot{\psi}_t\|,$$

where $\|\dot{\psi}_t\| = \sup_{x\in\Gamma} ||| \frac{d}{dt}(\psi_t x) |||$ *and* $|\Gamma|$ *means the area of* Γ *which is measured by* *the surface element induced from $d\lambda$ and the metric $|||\cdot|||$, i.e. if $\Gamma(\varepsilon)$ is the set of points whose distance from Γ measured by $|||\cdot|||$ is less than ε, then*

$$|\Gamma|=\lim_{\varepsilon\to 0}\frac{|\Gamma(\varepsilon)|}{2\varepsilon}.$$

Lemma 2. *For a given Hamiltonian system with interaction potential $U(q_1,\dots,q_{2n})$ and a total energy E we assume the conditions* (A1) *and* (A2) *are satisfied. Then for $S_a-S_b>0$ where S_a, $S_b\in\mathscr{R}_n(S)$ there exist some positive constants λ_3, $k'=k'(S_b, S_a)$ and $\gamma=\gamma(S_b, S_a)$ such that*

$$\frac{|\partial^{(-)}\Omega_{[S_b,S_a)}|}{|\Omega_{[S_b,S_a)}|}<k'n^{\lambda_3}e^{-\gamma n}.$$

Proofs of these lemmas will be given in section 3. Now we come to the stage to prove our theorem.

Proof of theorem. We estimate the size of the exceptional set $E(\Omega_{[S_b,S_a)})$ of initial conditions which cause the entropy to decrease from S_b, namely the set of initial conditions in $\Omega_{[S_b,S_a)}$ from which the lower boundary $\partial^{(-)}\Omega_{[S_b,S_a)}$ can be reached within time T:

$$E(\Omega_{[S_b,S_a)})=\{\omega\in\Omega_{[S_b,S_a)};\ T_t\omega\in\partial^{(-)}\Omega_{[S_b,S_a)}\quad\text{for some } |t|<T\}.$$

From lemma 1 we obtain

$$|E(\Omega_{[S_b,S_a)})|<2T|\partial^{(-)}\Omega_{[S_b,S_a)}|\ \|\dot{T}_t\|.$$

Using lemma 2 we obtain under the condition (A1) and (A2)

$$\frac{|E(\Omega_{[S_b,S_a)})|}{|\Omega_{[S_b,S_a)}|}<2Tk'n^{\lambda_1+\lambda_3}e^{-\gamma n}.$$

Now we can take α, β and $k>0$ which are independent of n but depending on S_b, S_a such that

$$e^{\beta n}=T\quad\text{and}\quad 2Tk'n^{\lambda_1+\lambda_3}e^{-\gamma n}<ke^{-\alpha n}$$

where $\gamma-\beta>0$ and $\alpha<\gamma-\beta$. From

$$\{\omega\in\Omega_{[S_b,S_a)};\ S(T_t\omega)\geqq S_b\ \text{ for } |t|<e^{\beta n}\}\supset\Omega_{[S_b,S_a)}-E(\Omega_{[S_b,S_a)}),$$

we obtain the desired result.

3. Proofs of lemmas.

Proof of lemma 1. Notice that for any positive integer L

$$\bigcup_{|t|<T}\psi_t\Gamma=\bigcup_{k=-L}^{L-1}\psi_{kT/L}\Big(\bigcup_{0<t<T/L}\psi_t\Gamma\Big).$$

So we have

$$|\bigcup_{|t|<T}\psi_t\Gamma|<\sum_{k=-L}^{L-1}|\psi_{kT/L}(\bigcup_{0<t<T/L}\varphi_t\Gamma)|=2L|\bigcup_{0<t<T/L}\psi_t\Gamma|,$$

here we use the ψ_t-invariance of the measure $d\lambda$. And clearly for any $\varepsilon>0$

$$|\bigcup_{0<t<\varepsilon}\psi_t\Gamma|\leqslant\varepsilon|\Gamma|\,\|\dot{\psi}_t\|+o(\varepsilon).$$

From these inequalities we get the result.

Proof of lemma 2. The entropy we consider is given by

$$S(\omega)=-\frac{x}{2n}\log\frac{x}{2n}-\left(1-\frac{x}{2n}\right)\log\left(1-\frac{x}{2n}\right)$$

where

$$x=\#\{i;\,(p_i,q_i)\in\mu_+\}.$$

We only need to consider the case $x\leqq n$ hereafter because of the symmetry of the function $h(y)=-y\log y-(1-y)\log(1-y)$ for $0\leqq y\leqq 1$.

We divide the energy surface Ω_E into 2^{2n} cells $C(\varepsilon_1,\dots,\varepsilon_{2n})$ with $2n$ suffixes $(\varepsilon_1,\dots,\varepsilon_{2n})$ defined by ($\varepsilon_i=0$ or 1)

$$C(\varepsilon_1,\dots,\varepsilon_{2n})=\{(p,q)\in\Omega_E;\,\varepsilon_i=\varepsilon(p_i)\qquad\text{for all}\quad i\}$$

where

$$\varepsilon(p_i)=\begin{cases}1 & \text{if}\quad p_i\in\boldsymbol{R}_+^f\\ 0 & \text{if}\quad p_i\in\boldsymbol{R}_-^f\end{cases}$$

We remark that when a phase point on Ω_E is in a certain cell $C(\varepsilon_1,\dots,\varepsilon_{2n})$ then $x=\sum_{i=1}^{2n}\varepsilon_i$. The boundary of a cell $C(\varepsilon_1,\dots,\varepsilon_{2n})$, $\partial C(\varepsilon_1,\dots,\varepsilon_{2n})$ is given by (except higher codimensional submanifolds)

$$\partial C(\varepsilon_1,\dots,\varepsilon_{2n})=\bigcup_{j=1}^{2n}\partial^j C(\varepsilon_1,\dots,\varepsilon_{2n})$$

where

$$\partial^j C(\varepsilon_1,\dots,\varepsilon_{2n})=\{(p,q)\in\Omega_E;\,\varepsilon(p_i)=\varepsilon_i,\ p_i^1\neq 0\quad\text{for } i\neq j\quad\text{and}\quad p_j^1=0\}.$$

Now we define the lower boundary $\partial^{(-)}C(\varepsilon_1,\dots,\varepsilon_{2n})$ of a cell $C(\varepsilon_1,\dots,\varepsilon_{2n})$ by

$$\partial^{(-)}C(\varepsilon_1,\dots,\varepsilon_{2n})=\bigcup_{\substack{(\varepsilon_1',\dots,\varepsilon_{2n}')\\ \sum_{i=1}^{2n}\varepsilon_i'=\sum_{i=1}^{2n}\varepsilon_i-1\\ \sum_{i=1}^{2n}|\varepsilon_i-\varepsilon_i'|=1}}\partial C(\varepsilon_1,\dots,\varepsilon_{2n})\cap\partial(\varepsilon_1',\dots,\varepsilon_{2n}')\quad\text{for }\sum_{i=1}^{2n}\varepsilon_i\leqslant n$$

$$= \bigcup_{\substack{(\varepsilon'_1,\ldots,\varepsilon'_{2n}) \\ \sum_{i=1}^{2n} \varepsilon'_i = \sum_{i=1}^{2n} \varepsilon_i + 1 \\ \sum_{i=1}^{2n} |\varepsilon_i - \varepsilon'_i| = 1}} \partial C(\varepsilon_1,\ldots,\varepsilon_{2n}) \cap \partial C(\varepsilon'_1,\ldots,\varepsilon'_{2n}) \quad \text{for } \sum_{i=1}^{2n} \varepsilon_i \geqslant n.$$

The upper boundary $\partial^{(+)}C(\varepsilon_1,\ldots,\varepsilon_{2n})$ of a cell is defined similarly.

Then the entropy band $\Omega_{[S_b,S_a)}$ for $S_b < S_a$ in $\mathscr{R}_n(S)$ is given by

$$\Omega_{[S_b,S_a)} = \bigcup_{\frac{n-x}{n} \in (a,b]} C_x \cup C_{2n-x}$$

where parameters a, b ($0 \leqq a$, $b \leqq 1$) are related to S_a, S_b through

$$h\left(\frac{1}{2}(1-a)\right) = S_a \quad \text{and} \quad h\left(\frac{1}{2}(1-b)\right) = S_b$$

and C_x is defined by

$$C_x = \bigcup_{\sum_{i=1}^{2n} \varepsilon_i = x} C(\varepsilon_1,\ldots,\varepsilon_{2n}).$$

For the lower boundary of the entropy band, we get

$$\partial^{(-)}\Omega_{[S_b,S_a)} = \partial^{(-)}C_{n-bn} \cup \partial^{(-)}C_{n+bn}$$

where

$$\partial^{(-)}C_x = \bigcup_{\sum_{i=1}^{2n} \varepsilon_i = x} \partial^{(-)}C(\varepsilon_1,\ldots,\varepsilon_{2n})$$

To estimate the ratio $|\partial^{(-)}\Omega_{[S_b,S_a)}|/|\Omega_{[S_b,S_a)}|$, notice that the sizes $|C(\varepsilon_1,\ldots,\varepsilon_{2n})|$, $|\partial(\varepsilon_1,\ldots,\varepsilon_{2n})|$ and $|\partial C^j(\varepsilon_1,\ldots,\varepsilon_{2n})|$ are independent of $(\varepsilon_1,\ldots,\varepsilon_{2n})$ and j. So we denote these by $|C|$, $|\partial C|$ and $|\partial^\circ C|$ respectively. Then we obtain,

$$\begin{aligned}
|\partial^{(-)}\Omega_{[S_b,S_a)}| &= |\partial^{(-)}C_{n-bn}| + |\partial^{(-)}C_{n+bn}| \\
&= \sum_{\sum_{i=1}^{2n} \varepsilon_i = n-bn} |\partial^{(-)}C(\varepsilon_1,\ldots,\varepsilon_{2n})| + \sum_{\sum_{i=1}^{2n} \varepsilon'_i = n+bn} |\partial^{(-)}C(\varepsilon'_1,\ldots,\varepsilon'_{2n})| \\
&= \binom{2n}{n-bn}(n-bn)|\partial^0 C| + \binom{2n}{n+bn}(2n-(n+bn))|\partial^0 C| \\
&= 2n(1-b)\binom{2n}{n+bn}|\partial^0 C|
\end{aligned}$$

And clearly

$$|C_{n-an-1}| < |\Omega_{[S_b,S_a)}|$$

where

$$|C_{n-an-1}| = \binom{2n}{n+an+1} |C|.$$

Therefore we obtain

$$\frac{|\partial^{(-)} \Omega_{[S_b, S_a)}|}{|\Omega_{[S_b, S_a)}|} < \frac{2n(1+a)(1-b)}{1-a} Q(a, b) \frac{|\partial^0 C|}{|C|}$$

where

$$Q(a, b) = \binom{2n}{n+bn} \Big/ \binom{2n}{n+an}$$

Using the Stirling formula, we get

$$Q(a, b) \sim e^{(f(a)-f(b))n} \sqrt{\frac{1-a^2}{1-b^2}}$$

where $f(y) = (1+y)\log(1+y) + (1-y)\log(1-y)$, $0 \leqq y \leqq 1$, is a monotone increasing function. As will be shown in the appendix, we have

$$\frac{|\partial^0 C|}{|C|} = \frac{2\sigma^{2fn-2}}{\sigma^{2fn-1}} \frac{\int_D dq R(q)^{2fn-3}}{\int_D dq R(q)^{2fn-2}}.$$

From the condition (A2) we obtain

$$\frac{|\partial^0 C|}{|C|} = \frac{2\sigma^{2fn-2}}{\sigma^{2fn-1}} \frac{1}{\kappa(E; H)} < n^{\lambda_2+2}.$$

Finally we have

$$\frac{|\partial^{(-)} \Omega_{[S_b, S_a)}|}{|\Omega_{[S_b, S_a)}|} < 2\sqrt{\frac{(1+a)^3(1-b)}{(1-a)(1+b)}}\, n^{\lambda_2+3} e^{-(f(b)-f(a))n}.$$

4. Example.

In this section we give an example which satisfies the condition (A2). To this end we divide the integration region $D = \{q \in V^{2n};\ E - U(q) \geqq 0\}$ into D_1 and D_2 where $D_1 = \{q \in V^{2n};\ E > e \geqq U(q)\}$ and $D_2 = D \backslash D_1$ for some e smaller than the total energy E. Then

$$\begin{aligned} \frac{1}{\kappa(E; H)} &< \frac{\left(1 + \frac{|D_2|}{|D_1|}\right) \int_{D_1} dq [2m(E-U)]^{fn-\frac{3}{2}}}{\int_{D_1} dq [2m(E-U)]^{fn-1}} \\ &\leqslant \frac{1}{\sqrt{2m(E-e)}} \frac{|D|}{|D_1|}. \end{aligned}$$

To obtain a regorous simple result we consider a class of pair potentials which depend on the distance between each pair of particles. The potentisl for this class is represented by

$$U(q_1,\dots,q_{2n})=\sum_{1<i<j<2n}\Phi(r_{ij})$$

where $r_{ij}=|q_i-q_j|$ for q_i, $q_j\in V$ and

$$\Phi(r)=n^{-\lambda}\phi(n^{\delta}r)\quad (r>0),$$

here λ and δ are some scaling factors for n and $\phi(r)$ is a smooth function with the range $\{R\cup\infty\}$.

Then we obtain the following proposition which gives a sufficient condition for the assumption (A2).

Proposition. *Assume that there exists $r_0>0$ such that*

$$\phi(r)\begin{cases}\geqq 0 & \text{if } r\leqq r_0\\ \leqq 0 & \text{if } r>r_0\end{cases}$$

and that $\delta>2/3$, $E>0$, then the assumption on the kinetic activity (A2) *is satisfied.*

Proof of proposition. Let $e=0$, then $D_1=\{q\in V^{2n};\ U(q)\leqq 0\}$. Setting $v=\frac{4\pi}{3}\left(\frac{2r_0}{n^{\delta}}\right)^3$,
we get

$$\frac{|D_1|}{|D|}>\frac{\prod_{k=0}^{2n-1}|V-kv|}{|V|^{2n}}=\exp\left[\sum_{k=0}^{2n-1}\log\left(1-k\frac{|v|}{|V|}\right)\right]$$

$$>\exp\left(-\frac{2|v|}{|V|}\sum_{k=0}^{2n-1}k\right)>\exp\left(-\frac{128\pi r_0^3}{3|V|}\frac{n^2}{n^{3\delta}}\right).$$

Since $\delta>2/3$ and n is large, this concludes the proof.

We remark that we can obtain the same result, even if we take the boundary condition, mentioned in the begining of section 2, into the consideration.

This proposition says that the condition for the kinetic activity may be satisfied for the dilute gases.

5. Discussion.

Our theorem means that for a nonequilibrium state ω, the time evolution of the entropy $S(T_t\omega)$ takes the "local minimum" at $t=0$ for a long time interval $(-T, T)$, $T=e^{\beta n}$. This fact coincides with the property of H-curve, pointed out by Ehrenfest [2]. Therefore in this sense the Boltzmann entropy may behave with "fluctuation" as if "it is always taking local minimum and has a tendency to increase". Consequently when the number of particles becomes infinitely large, the dynamical system enable to have the property that the entropy does not decrease, which is compatible with the reversibility and Poincare's recurrence theorem.

It would be interesting to investigate whether there exists a system which does not satisfy the condition (A2) of theorem, that is, whose index of the kinetic activity is extremely small, say $\kappa(E; H) \sim e^{-n}$, because in such a case it is difficult to justify the statement that the entropy should increase. As we mentioned in a previous section, the condition for the kinetic activity is satisfied in the case of the dilute gases. We notice here that for a system with condenced density and extremely small kinetic energy compared with potential one this condition may be false and so that the Boltzmann entropy may actually decrease. This circumstance seems to relate profoundly to the arguments about the adequacy of Boltzmann's equation for dense gases.

Our theorem, however, is proved only for the simple partition $\mathscr{P}_0$. So concerning to the dependence on the partition, several problems are left. The first one is to extend our result to more general cases, in which the partitions are defined in momentum and also configuration space, and the second one is to check the dependence on the choice of the partition and on its refinements. We note here only on the first one partially; for the finite partition into rectangular parallelopiped cells with the same size cut along the coordinates (p, q), we obtain a similar formula on $|\partial^{(-)}\Omega_{[s_b,s_a)}|/|\Omega_{[s_b,s_a)}|$, but rigorous estimates on the expressions which correspond to $|\partial^{(-)}C|$, $|C|$ in this paper are very complicated. However for the partition only in momentum space, like mentioned above, one could obtain a similar result. (At least in some case of the "star-like" partition in momentum space, we can show the similar result.)

Appendix.

We notice that $|C|$ is given by $|\Omega_E|/2^{2n}$. To calculate $|\Omega_E|$, we remark that Ω_E is also given by

$$\Omega_E = \{p_1^1 = \pm\sqrt{R(q)^2 - \underset{\sim}{p}^2},\ \underset{\sim}{p}^2 \leqq R(q)^2,\ q \in D\}$$

where

$$R(q)^2 = 2m(E - U(q)) \quad \text{and}$$

$$\underset{\sim}{p} = (p_1^2, p_1^3, \dots, p_{2n}^1, \dots, p_{2n}^f).$$

Then

$$|\Omega_E| = 2\int_{\substack{q \in D \\ \underset{\sim}{p}^2 < R(q)^2}} \frac{d\Sigma_E}{\|\mathrm{Grad}\, H\|}$$

where

$$\|\mathrm{Grad}\, H\| = \left[\left|\frac{\partial H}{\partial q}\right|^2 + \left|\frac{\partial H}{\partial p}\right|^2\right]^{1/2}$$

and the surface element $d\Sigma_E$ of the energy surface is given by

$$d\Sigma_E = \left[1 + \left|\frac{\partial}{\partial \underset{\sim}{p}} p_1^1(\underset{\sim}{p}, q)\right|^2 + \left|\frac{\partial}{\partial q} p_1^1(\underset{\sim}{p}, q)\right|^2\right]^{1/2} d\underset{\sim}{p}dq.$$

Therefore

$$|\Omega_E| = m \int_{q \in D} dq\ R(q)^{-1} \int_{\underset{\sim}{p}^2 < R(q)^2} d\underset{\sim}{p} \frac{2R(q)}{(R(q)^2 - \underset{\sim}{p}^2)^{1/2}}.$$

Let σ^{m-1} be the surface area of the unit sphere in $\boldsymbol{R}^m$, i.e. $\sigma^{m-1} = |\{(x_1, \ldots, x_m);\ x_1^2 + \cdots + x_m^2 = 1\}|$. Then

$$|C| = \frac{\sigma^{2fn-1}}{2^{2n}} m \int_{q \in D} dq\ R(q)^{2fn-2}$$

In the same way as above we obtain

$$|\partial C| = 2n |\partial^0 C| = \frac{2n\sigma^{2fn-2}}{2^{2n-1}} m \int_{q \in D} dq R(q)^{2fn-3}.$$

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