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The conditional entropy in the microcanonical ensemble

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The existence of the configurational microcanonical conditional entropy in classical statistical mechanics is proved in the thermodynamic limit for a class of long-range multiparticle observables. This result generalizes a theorem of Lanford for finite range observables.

Although a considerable amount of research has been directed in recent years toward proving the existence of the thermodynamic limit for the classical ensembles, the microcanonical ensemble for long-range interactions has presented certain difficulties. In this article we provide a proof of the existence of the configurational conditional entropy for a class of systems including long-range interactions falling off in ν dimensions faster than $1/r^\nu$.

Griffiths, using arguments of Fisher,^{1,2} has outlined proofs of the existence of the microcanonical entropy for variously tempered two-body interactions. There the microcanonical energy is studied as a function of the entropy, and the entropy is recovered implicitly after the infinite volume limit has been taken. Similar results for two-body interactions were obtained by Minlos and Povzner.³

Lanford⁴ has pointed out that methods of Ruelle⁵ can be employed to obtain the entropy directly, and has used this approach to prove the existence of the configurational conditional entropy for strictly finite-range observables.

We use the Lanford approach to extend the existence theorem to observables with long-range behavior.

1. LIMIT ALONG A SPECIAL SEQUENCE OF CUBES

Let T^ν designate either the ν -dimensional lattice Z^ν or ν -dimensional real Euclidean space \mathbb{R}^ν with counting or Lebesgue measure μ , and denote the corresponding phase space by \mathcal{G} , $\mathcal{G} = \bigcup_{n=1}^{\infty} (T^\nu)^n$. The extension of μ to $(T^\nu)^n$ and \mathcal{G} will also be written μ . If $Q_i \in \mathcal{G} \cap (T^\nu)^{n_i}$, $Q_i = (q_{i1}, \dots, q_{in_i})$, $i = 1, 2$, write $N(Q_i) = n_i$, $q_{ij} \in Q_i$, and $d(Q_1, Q_2) = \inf\{\bar{d}(q_1, q_2) \mid q_i \in Q_i\}$, where $\bar{d}: T^\nu \times T^\nu \rightarrow \mathbb{R}$ is the Euclidean metric. Let \mathcal{J} be the set of bounded, measurable subsets of T^ν , and \mathcal{C}_t , the set of bounded open convex subsets of \mathbb{R}^t , $t \in Z_+$. If $J \in \mathcal{C}_t$ and $\epsilon > 0$, then $J^\epsilon = \{x \in J \mid \|x - y\| > \epsilon, \forall y \in \mathbb{R}^t/J\}$ is the ϵ -contraction of J , and $J^{-\epsilon} = \{x \in \mathbb{R}^t \mid \|x - y\| < \epsilon \text{ for some } y \in J\}$.

Definition 1.1: The real linear space \mathcal{A}_t^λ of t -valued observables, $t \in Z_+$ and $\lambda \in \mathbb{R}$, is the set of μ -measurable functions $f: \mathcal{G} \rightarrow \mathbb{R}^t$ satisfying the following:

- (i) $f(Q+q) = f(Q)$, $Q \in \mathcal{G}$, $q \in T^\nu$, and $Q+q = \{p \in T^\nu \mid p-q \in Q\}$;
- (ii) $f(Q) = f(Q')$ if Q' is a permutation of Q ;

(iii) there exist $A > 0$ and $R_0 > 0$ such that, for all $m \in Z_+$ and $Q_1, \dots, Q_m \in \mathcal{G}$, $d(Q_i, Q_j) \geq r \geq R_0$ for all $i \neq j$ implies

$$\left\| f(Q_1, \dots, Q_m) - \sum_{i=1}^m f(Q_i) \right\| \leq \frac{A}{r^\lambda} \left(\sum_{i=1}^m N(Q_i) \right)^2.$$

For $\Lambda \in \mathcal{J}$, $J \in \mathcal{C}_t$, $n \in Z_+$, and $f \in \mathcal{A}_t^\lambda$, the conditional phase space volume V_f is

$$V_f(\Lambda, n, J) = (1/n!) \mu\{Q \in \Lambda^n \mid (1/n)f(Q) \in J\}.$$

The vector-valued observable f is to be viewed as a set of t translation-invariant symmetric scalar-valued observables, with a decrease condition (tempering) for each at large distances. For example, tempering would require a pair potential interaction generating a Hamiltonian to fall off at least as fast as $r^{-\lambda}$. Since the observable f will be fixed, the subscript on V will be dropped. Also, throughout it will be necessary to assume that $\lambda > \nu$.

Proposition 1.2: (a) If $J \in \mathcal{C}_t$ and $\Lambda \subset \Lambda'$, $\Lambda, \Lambda' \in \mathcal{J}$, then $V(\Lambda', n, J) \geq V(\Lambda, n, J)$.

(b) If $\{\Lambda_i\}_{i=1}^m \subset \mathcal{J}$, $d(\Lambda_i, \Lambda_j) \geq r \geq R_0$ for $i \neq j$, $n = \sum_{i=1}^m n_i$, $n_i \in Z_+$, and $\{J_i\}_{i=1}^m \subset \mathcal{C}_t$, then

$$V\left(\bigcup_{i=1}^m \Lambda_i, \sum_{i=1}^m n_i, \sum_{i=1}^m \left(\frac{n_i}{n}\right) J_i\right) \geq \prod_{i=1}^m V(\Lambda_i, n_i, J_i^{A_i^{m-\lambda}}).$$

Proof: The first part is obvious. If $Q_i \in \Lambda_i^{n_i}$, then for $J = \sum_{i=1}^m (n_i/n) J_i$, $(1/n)f(Q_i) \in J_i^{A_i^{m-\lambda}}$ implies $(1/n)f(Q_1, \dots, Q_m) \in J$ by 1.1 (iii), since

$$\frac{1}{n} \sum_{i=1}^m f(Q_i) \in \sum_{i=1}^m \left(\frac{n_i}{n}\right) J_i^{A_i^{m-\lambda}} = J^{A^{m-\lambda}}.$$

Hence

$$\left\{ (Q_1, \dots, Q_m) \mid Q_i \in \Lambda_i^{n_i} \text{ and } \frac{1}{n} f(Q_i) \in J_i^{A_i^{m-\lambda}} \right\}$$

$$\subset \left\{ Q \in \left(\bigcup_{i=1}^m \Lambda_i\right)^n \mid \frac{1}{n} f(Q) \in \sum_{i=1}^m \left(\frac{n_i}{n}\right) J_i \right\}.$$

Define the density $\rho = n/\mu(\Lambda)$, the specific volume $v = 1/\rho$, and $l_\nu = v^{1/\nu}$. For $\epsilon = \lambda - \nu > 0$ as in 1.1 (ii), $\kappa \in (0, 1)$, and $m \in Z_+$, let $\theta_\kappa = 2^{(\nu+\kappa\epsilon)/\lambda}$, $\varphi_\kappa = [1 - (2^\nu/\theta_\kappa^\lambda)]^{-1}$, $R_\kappa = R_0(2 - \theta_\kappa)^{-1}$, $R_{\kappa,m} = \theta_\kappa^m R_0$, and $\Delta_{\kappa,m} = A \varphi_\kappa 2^{(m+1)\nu}/R_{\kappa,m}^\lambda$. Denote the cube $\Lambda_{\kappa,m}(v) = \{q = (q_1, \dots, q_\nu) \in T^\nu \mid 0 < q_k < 2^m l_\nu - \theta_\kappa^m R_{\kappa,m}, k = 1, \dots, \nu\}$.

The reasons for choosing $\Lambda_{\kappa,m}(v)$ and $R_{\kappa,m}$ in this manner will be apparent from Proposition 1.3. In particular, φ_κ is chosen to make valid the last equality in the proof of that proposition. Note that as $m \rightarrow \infty$ $\Delta_{\kappa,m}$ goes to zero as $2^{-\kappa \epsilon m}$, and $J^{\Delta_{\kappa,m}} \rightarrow J$. The parameter κ is specified, since later some control will be needed over the rate of convergence of $\Delta_{\kappa,m}$ to zero.

Proposition 1.3: If $J \in C_t$, then

$$\bigvee(\Lambda_{\kappa,m+1}(v), 2^{(m+1)\nu}, J^{\Delta_{\kappa,m+1}}) \geq \left\{ \bigvee(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta_{\kappa,m}}) \right\}^{2^\nu}$$

Proof: Since $R_{\kappa,m} = (2^{m+1}l_v - \theta_{\kappa}^{m+1}R_\kappa) - 2(2^m l_v - \theta_{\kappa}^m R_\kappa)$, 2^ν disjoint translates of $\Lambda_{\kappa,m}(v)$ with mutual separation equal to or greater than $R_{\kappa,m}$ can be placed inside $\Lambda_{\kappa,m+1}(v)$. Further,

$$(J^{\Delta_{\kappa,m+1}})^{A^{2^{(m+1)\nu}/R_{\kappa,m}}} = J^{\Delta_{\kappa,m}}$$

The proof is completed using 1.2.

Corollary 1.4:

$$\begin{aligned} & \frac{1}{2^{(m+1)\nu}} \log \bigvee(\Lambda_{\kappa,m+1}(v), 2^{(m+1)\nu}, J^{\Delta_{\kappa,m+1}}) \\ & \geq \frac{1}{2^{m\nu}} \log \bigvee(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta_{\kappa,m}}) \end{aligned}$$

and the limit as $m \rightarrow \infty$ is equal to the supremum over $m \in Z_+$.

Definition 1.5: For $J \in C_t$ and $x \in \mathbb{R}^t$, let

$$S_\kappa(v, J) = \lim_{m \rightarrow \infty} \frac{1}{2^{m\nu}} \log \bigvee(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta_{\kappa,m}})$$

and

$$s_\kappa(v, x) = \inf_{x \in J \in C_t} \{S_\kappa(v, J)\}.$$

Proposition 1.6: (i) If $J \subset J'$, $J, J' \in C_t$, then $S_\kappa(v, J) \leq S_\kappa(v, J') \leq 1 + \log v$.

(ii) If $\{J_i\}_{i=1}^k \subset C_t$, $J_0 = \bigcup_{i=1}^k J_i \in C_t$, and for $\Delta > 0$ sufficiently small, $\bigcup_{i=1}^k J_i^\Delta = J_0^\Delta$, then $S_\kappa(v, \bigcup_{i=1}^k J_i) = \sup_{1 \leq i \leq k} S_\kappa(v, J_i)$.

(iii) If $J \in C_t$, then $S_\kappa(v, J) = \sup\{S_\kappa(v, \hat{J}) \mid \hat{J} \in C_t, \hat{J} \subset J\}$.

(iv) $S_\kappa(v, J) = \sup_{x \in J} S_\kappa(v, x)$.

Proof: Routine, using 1.2 and properties of μ .

Corollary 1.7: (i) $x \rightarrow s_\kappa(v, x)$ is upper semicontinuous and concave on \mathbb{R}^t .

(ii) $v - s_\kappa(v, x)$ is nondecreasing and concave on \mathbb{R}_+ , and continuous on (v_x, ∞) , where $v_x = \inf\{v \mid s_\kappa(v, x) > -\infty\}$.

When the tempering condition in the definition of A_t^λ is replaced by a finite range condition (additivity: $A=0$), then the interior of Γ_κ is nonempty if the components of f are linearly independent. More generally, a sort of asymptotic openness is required.

Proposition 1.8: Let $\Omega_\kappa(v)$ be the convex set

$$\Omega_\kappa(v) = \{x \in \mathbb{R}^t \mid s_\kappa(v, x) > -\infty\},$$

and, for $m \in Z_+$, let $E_m(v) = \text{ess range } ((1/2^{m\nu})f_{\kappa,m})$, where $f_{\kappa,m}$ is the restriction of f to $[\Lambda_{\kappa,m}(v)]^{2^{m\nu}}$. Write

$$\lim_{n \rightarrow \infty} s. E_m(v)$$

$$= \{x \in \mathbb{R}^t \mid 0 \cap E_m(v) \neq \emptyset \text{ for infinitely many } m, \text{ for each open } 0 \subset \mathbb{R}^t, x \in 0\}.$$

Then

$$\Omega_\kappa(v)^* = \lim_{m \rightarrow \infty} s. E_m(v).$$

Proof: If $x_0 \notin \Omega_\kappa(v)^*$, then there exists $J \in C_t$ such that $x_0 \in J$ and $S_\kappa(v, J) = -\infty$, hence $J^{\Delta_{\kappa,m}} \cap E_m(v) = \emptyset$ and $x_0 \notin J^{\Delta_{\kappa,m}}$ for m sufficiently large. Therefore, $x_0 \notin \lim_{m \rightarrow \infty} s. E_m(v)$.

On the other hand, $x_0 \notin \lim_{m \rightarrow \infty} s. E_m(v)$ implies $J \cap E_m(v) = \emptyset$ for some $J \in C_t$, $x_0 \in J$, and all sufficiently large m . Passing to the contraction $J^{\Delta_{\kappa,m}}$ gives the desired result.

Definition 1.9: We say that f is asymptotically open if there exists $v > 0$ and $\kappa = \kappa$ such that $(\lim_{m \rightarrow \infty} s. E_m(v))^0 \neq \emptyset$. We denote by $v_0(\kappa)$ the infimum over all such v for any $\kappa \leq \kappa$. In the remainder we will always assume that $\kappa \leq \kappa$.

If f is asymptotically open and $v > v_0(\kappa)$, then $\Omega_\kappa(v)^0 \neq \emptyset$. Let $\Gamma_\kappa = \Gamma_\kappa(f)$ be the set $\{(v, x) \in \mathbb{R}_+ \times \mathbb{R}^t \mid s_\kappa(v, x) > -\infty\}$.

Corollary 1.10: (i) Γ_κ^0 is convex.

(ii) If f is asymptotically open, then Γ_κ^0 is nonempty and dense in Γ_κ .

(iii) $(v, x) \rightarrow s_\kappa(v, x)$ is continuous and concave on Γ_κ^0 .

Corollary 1.11: If f is asymptotically open and $0 < v < v_0(\kappa)$, then $\Omega_\kappa(v) = \emptyset$. Hence $v_0(\kappa) = \inf_x v_x$.

2. INDEPENDENCE OF THE PARAMETER

We shall show in this section that the contraction parameter κ can be removed, and that the result coincides with the conditional entropy defined without contractions, at least for the limit taken along a special sequence of cubes.

Lemma 2.1: Let $f: \mathbb{R}^t \rightarrow \mathbb{R} \cup \{-\infty, \infty\}$ be upper semicontinuous and concave, $J_1, J_2 \in C_t$ with $J_1 \cap J_2 \neq \emptyset$, $f(J_1 \cap J_2) \cap \mathbb{R} \neq \emptyset$, and $\{d_i\}_{i=1}^\infty$ a sequence of positive real numbers with $d_i \rightarrow 0$. Then

$$\inf_i \sup_{x \in J_1^{-d_i} \cap J_2} f(x) = \sup_{x \in J_1 \cap J_2} f(x).$$

Proof: Since $J^{-d_i} \supset J$,

$$\inf_i \sup_{x \in J_1^{-d_i} \cap J_2} f(x) \geq \sup_{x \in J_1 \cap J_2} f(x).$$

So assume $(J_1^{-d_i}/J_1) \cap J_2 \neq \emptyset$ for all i , $\sup_{x \in J_1 \cap J_2} f(x) < \infty$, and suppose

$$\inf_i \sup_{x \in J_1^{-d_i} \cap J_2} f(x) > \sup_{x \in J_1 \cap J_2} f(x) + \frac{3}{2}\epsilon, \quad \epsilon > 0.$$

Then, for each i ,

$$\sup_{x \in (J_1^{-d_i}/J_1) \cap J_2} f(x) > \sup_{x \in J_1 \cap J_2} f(x) + \frac{3}{2}\epsilon.$$

Let $v_i' \in (J_1^{-d_i}/J_1) \cap J_2$ be such that

$$f(y_i) > \sup_{x \in (J_1^{d_i} \times J_2) \cap J_2} f(x) - \epsilon/2$$

and $\{y_i\}_{i=1}^\infty$ a subsequence convergent to $y \in \partial(J_1 \cap J_2)$. If $z_i \rightarrow y$, by upper semicontinuity,

$$f(y) \geq \limsup_{i \rightarrow \infty} f(z_i) \geq \limsup_{i \rightarrow \infty} f(y_i) \geq \sup_{x \in J_1 \cap J_2} f(x) + \epsilon$$

and by concavity

$$\sup_{x \in (J_1 \cap J_2)^c} f(x) = \sup_{x \in J_1 \cap J_2} f(x),$$

which yields a contradiction.

Definition 2.2: For $v > 0$ and $\kappa \in (0, \kappa)$, let $\tilde{C}_t(v, \kappa) = \{J \in \tilde{C}_t(\{v\} \times J) \cap \Gamma_\kappa \neq \emptyset \text{ or } d(\{v\} \times J, \Gamma_\kappa) > 0\}$. For $J \in \tilde{C}_t(v, \kappa)$ and $x \in \mathbb{R}^t$, define

$$S_{\kappa,0}(v, J) = \lim_{m \rightarrow \infty} \frac{1}{2^{m\nu}} \log V(\Lambda_{\kappa,m}(v), 2^{m\nu}, J),$$

$$s_{\kappa,0}(v, x) = \inf_{x \in J \in \tilde{C}_t} S_{\kappa,0}(v, J),$$

and for $\kappa_1, \kappa_2 \in (0, \kappa)$, $\alpha > 0$,

$$S_{\kappa_1, \kappa_2, \alpha}(v, J) = \lim_{m \rightarrow \infty} \frac{1}{2^{m\nu}} \log V(\Lambda_{\kappa_1, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_2, m}})$$

Theorem 2.3: If $0 < v \neq v_0(\kappa_i)$, $\alpha > 0$, $\kappa_1, \kappa_2 \in (0, \kappa)$, and $J \in \tilde{C}_t(v, \kappa_1) \cap \tilde{C}_t(v, \kappa_2)$, then

$$(i) S_{\kappa_1,0}(v, J) = S_{\kappa_1}(v, J),$$

$$(ii) S_{\kappa_1}(v, J) = S_{\kappa_2}(v, J),$$

$$(iii) S_{\kappa_1, \kappa_2, \alpha}(v, J) = S_{\kappa_1}(v, J).$$

Proof: For each $d > 0$ there exists a positive integer $m(d)$ satisfying

$$(1/2^{m\nu}) \log V(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq (1/2^{m\nu}) \log V(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{-d+\Delta_{\kappa,m}})$$

for $m > m(d)$. Hence, if $\{d_i\}_{i=1}^\infty$ is a sequence of positive numbers with $d_i \rightarrow 0$,

$$\limsup_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq \inf_i S_{\kappa}(v, J^{-d_i}).$$

Now, by Proposition 1.6(iv) and the concavity of $x \rightarrow s_{\kappa}(v, x)$,

$$S_{\kappa}(v, J^{-d_i}) = \sup\{s_{\kappa}(v, x) \mid x \in J^{-d_i} \cap \Omega_{\kappa}(v)^0\}.$$

Therefore, for $(\{v\} \times J) \cap \Gamma_{\kappa}^0 \neq \emptyset$, by 1.7 and 2.1, $\inf_i S_{\kappa}(v, J^{-d_i}) = S_{\kappa}(v, J)$, and so

$$\limsup_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq S_{\kappa}(v, J).$$

In the case $d(\{v\} \times J, \Gamma_{\kappa}) > 0$, if δ satisfies $(\{v\} \times J^{-\delta}) \cap \Gamma_{\kappa} = \emptyset$, then $S_{\kappa}(v, J^{-\delta}) = -\infty$, so that $S_{\kappa}(v, J) = -\infty$.

Assuming $\kappa_2 > \kappa_1$ and noting $\Lambda_{\kappa_2, m}(v) \subset \Lambda_{\kappa_1, m}(v)$, obtain $S_{\kappa_2,0}(v, J) \leq S_{\kappa_1,0}(v, J)$. On the other hand, letting $0 < v' < v$ if $v < v_0(\kappa_1)$, or $v_0(\kappa_1) < v' < v$ otherwise, compute

$$\lim_{m \rightarrow \infty} \frac{2^{m+1} l_v - \theta_{\kappa_2}^{m+1} R_{\kappa_2}}{2(2^m l_{v'})} = \frac{l_v}{l_{v'}} > 1,$$

so that 2^{ν} disjoint translates of the cube with sides $(0, 2^m l_{v'})$ can be placed inside $\Delta_{\kappa_2, m+1}(v)$ for all sufficiently large m , and hence 2^{ν} disjoint translates of $\Lambda_{\kappa_1, m}(v')$ with mutual separations equal to or greater than $R_{\kappa_1, m}$. Since

$$J^{\Delta_{\kappa_1, m+1}} \subset J^{\Delta_{\kappa_2, m+1}}$$

for sufficiently large m , therefore

$$V(\Lambda_{\kappa_2, m+1}(v), 2^{(m+1)\nu}, J^{\Delta_{\kappa_2, m+1}}) \geq [V(\Lambda_{\kappa_1, m}(v'), 2^{m\nu}, J^{\Delta_{\kappa_1, m}})]^{2^{\nu}}$$

and so

$$S_{\kappa_2}(v, J) \geq \sup_{v' < v} S_{\kappa_1}(v', J) = S_{\kappa_1}(v, J).$$

Thus (ii) follows from (i).

Finally, for $\kappa_2 > \kappa_1$, $d > 0$, and m sufficiently large,

$$V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\Delta_{\kappa_2, m}}) \geq V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}})$$

and

$$V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}}) \geq V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{d+\Delta_{\kappa_2, m}})$$

so that

$$S_{\kappa_2}(v, J) \geq \limsup_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}})$$

and

$$\liminf_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}}) \geq \sup_{d > 0} S_{\kappa_2}(v, J^d)$$

$$\geq \sup\{S_{\kappa_2}(v, \hat{J}) \mid \hat{J} \in \tilde{C}_t \text{ and } \hat{J} \subset J\} = S_{\kappa_2}(v, J).$$

If $\kappa_2 < \kappa_1$, then, for m large,

$$V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}}) \geq V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\Delta_{\kappa_2, m}})$$

so that

$$\liminf_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}}) \geq S_{\kappa_2}(v, J).$$

On the other hand,

$$S_{\kappa_2}(v, J) = S_{\kappa_2,0}(v, J) \geq \limsup_{m \rightarrow \infty} (1/2^{m\nu}) \log V(\Lambda_{\kappa_2, m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1, m}}).$$

Corollary 2.4: For all $v > 0$, $v \neq v_0(\kappa_1)$, $\kappa_1, \kappa_2, \kappa_3 \in (0, \kappa)$, and $x \in \mathbb{R}^t$,

$$S_{\kappa_1}(v, x) = S_{\kappa_2}(v, x) = S_{\kappa_3,0}(v, x).$$

Corollary 2.5: $\Gamma(f) = \Gamma_{\kappa}(f)$, $\tilde{C}_t(v) = \tilde{C}_t(v, \kappa)$, and $v_0 = v_0(\kappa)$ are independent of κ .

3. LIMIT ALONG GENERAL SEQUENCES

We wish to extend the results of the previous sections, derived for limits taken along the *standard* sequences of cubes $\{\Lambda_{\kappa, m}\}_{m=1}^\infty$, to limits along a more general sequence of domains.

For $\Lambda \in \mathcal{J}$ with boundary $\partial\Lambda$, let $V_{\partial}(\nu; \Lambda)$

$= \mu\{x \in T^d d(x, \partial\Lambda) \leq r\}$. A sequence $\{\Lambda_i\}_{i=1}^\infty \subset \mathcal{J}$ is said to tend to infinity in the sense of Fisher, $\Lambda_i \rightarrow \infty$ (Fisher) if $V(\Lambda_i) \rightarrow \infty$ and there exists an $i_0 \in \mathbb{Z}_+$ such that

$$\limsup_{\alpha \rightarrow 0} \sup_{i \geq i_0} V_\alpha(\alpha V(\Lambda_i)^{1/\nu}; \Lambda_i) / V(\Lambda_i) = 0.$$

Lemma 3.1¹: If $\Lambda \in \mathcal{J}$ is filled with cubes of edge-length d lying entirely within Λ , the volume remaining after maximal filling is less than $V_\alpha(\nu^{1/\nu} d; \Lambda)$.

Suppose $\{\Lambda_i\}_{i=1}^\infty \subset \mathcal{J}$, $\Lambda_i \rightarrow \infty$ (Fisher), and $\{n_i\}_{i=1}^\infty \subset \mathbb{Z}_+$ satisfy $\lim_{i \rightarrow \infty} V(\Lambda_i)/n_i = v \in (0, \infty)$. Then we will say that $\{(\Lambda_i, n_i)\}_{i=1}^\infty$ is a Fisher system tending to density $1/v$. In this case, let $\kappa, \kappa', \kappa'' \in (0, \kappa)$ be such that $\kappa'' > \kappa' > \kappa$ and $\kappa'' - \kappa' > \kappa$, for $n \in \mathbb{Z}_+$; let $m(n) = \lfloor ((\log_2 n)[v + \kappa'(\lambda - \nu)]^{-1}) \rfloor$, where $\lfloor x \rfloor$ is the greatest integer in x , and define $n_i = m_i 2^{m(n_i)\nu} + r_i$ with $0 \leq r_i < 2^{m(n_i)\nu}$ and

$$r_i = \sum_{j=0}^{m(n_i)-1} C_{ij} 2^{j\nu}$$

For $0 < v' < v$, let $\xi > 1$ satisfy $v' < \xi^\nu v' < v$, and write $\Lambda_m(\xi^\nu v')$, $m \in \mathbb{Z}_+$, for the cube in T^ν with edges $(0, 2^m \xi l_\nu)$. Finally, let \mathcal{J}_i be the number of cubes in a maximal filling of Λ_i with translates of cubes $\Lambda_{m(n_i)}(\xi^\nu v')$.

Lemma 3.2: For i sufficiently large, $m_i + \sum_{j=0}^{m(n_i)-1} C_{ij}$ disjoint translates of $\Lambda_{m(n_i)}(\xi^\nu v')$ may be placed inside Λ_i .

Proof: Observe

$$\lim_{i \rightarrow \infty} \frac{\mathcal{J}_i 2^{m(n_i)\nu}}{n_i} = \frac{v}{\xi^\nu v'} \lim_{i \rightarrow \infty} \frac{\mathcal{J}_i V(\Lambda_{m(n_i)}(\xi^\nu v'))}{V(\Lambda_i)}.$$

Therefore, if $\lim_{i \rightarrow \infty} \mathcal{J}_i V(\Lambda_{m(n_i)}(\xi^\nu v')) / V(\Lambda_i) = 1$, then $\lim_{i \rightarrow \infty} \mathcal{J}_i / m_i \geq v / \xi^\nu v'$, and so there exists $\xi \in \mathbb{R}$, $\xi^\nu v' / v < \xi < 1$ such that $\mathcal{J}_i > m_i + (\xi v / \xi^\nu v' - 1)m_i$ for all large enough i . Hence $m_i + \lfloor (m_i \xi v / \xi^\nu v' - m_i) \rfloor$ disjoint translates of $\Lambda_{m(n_i)}(\xi^\nu v')$ may be placed inside Λ_i , and the lemma follows from obvious estimates.

Using 3.1 for $i \geq i_0$ and

$$H(\alpha) = \sup_{i \geq i_0} V_\alpha(\alpha V(\Lambda_i)^{1/\nu}; \Lambda_i) / V(\Lambda_i),$$

$$1 - \frac{\mathcal{J}_i V(\Lambda_{m(n_i)}(\xi^\nu v'))}{V(\Lambda_i)} \leq \frac{V_\alpha(\nu^{1/\nu} 2^{m(n_i)} \xi l_\nu; \Lambda_i)}{V(\Lambda_i)} \leq H\left(\frac{\nu^{1/\nu} 2^{m(n_i)} \xi l_\nu}{V(\Lambda_i)^{1/\nu}}\right).$$

Choose $w \in \mathbb{R}$, $\xi l_\nu / l_\nu < w < 1$, so that, for i large, $V(\Lambda_i)^{1/\nu} > w l_\nu n_i^{1/\nu}$. Then $\xi l_\nu / V(\Lambda_i)^{1/\nu} < n_i^{1/\nu}$, and

$$H(\nu^{1/\nu} 2^{m(n_i)} \xi l_\nu / V(\Lambda_i)^{1/\nu}) \leq H(\nu^{1/\nu} n_i^{1/\nu} / (w \nu^{1/\nu} (\lambda - \nu)^{-1/\nu})).$$

But

$$\lim_{i \rightarrow \infty} n_i^{1/\nu} / (w \nu^{1/\nu} (\lambda - \nu)^{-1/\nu}) = 0.$$

Theorem 3.3: Suppose $\{(\Lambda_i, n_i)\}_{i=1}^\infty$ is a Fisher system tending to density $1/v$, $v \neq v_0$. Let $\{d_i\}_{i=1}^\infty$ be a sequence of nonnegative real numbers, $d_i \rightarrow 0$, $\kappa \in (0, \kappa)$, and $J \in \tilde{\mathcal{C}}_t(v)$. Then

$$\liminf_{i \rightarrow \infty} \frac{1}{n_i} \log \mathcal{V}(\Lambda_i, n_i, J^{\Delta_i}) \geq S_{\kappa,0}(v, J).$$

Proof: From 1.6 and 2.3, it is sufficient to show that there exists $\kappa'' \in (0, \kappa)$ such that for all $v_0 < v' < v$ and $\hat{J} \in \mathcal{C}_t$ with $\hat{J} \subset J$,

$$\liminf_{i \rightarrow \infty} (1/n_i) \log \mathcal{V}(\Lambda_i, n_i, J^{\Delta_i}) \geq S_{\kappa''}(v', \hat{J}).$$

Suppose $\kappa, \kappa', \kappa'' \in (0, \kappa)$ as before, Lemma 3.2. By that lemma, for sufficiently large i , $m_i + \sum_{j=0}^{m(n_i)-1} C_{ij}$ disjoint translates of $\Lambda_{\kappa'', m(n_i)}(\xi^\nu v')$ with mutual separation at least $\theta_{\kappa''}^{m(n_i)} R_0$ may be placed inside Λ_i . Therefore, for any $\tilde{J} \in \mathcal{C}_t$ and i sufficiently large,

$$\begin{aligned} \mathcal{V}_i &\equiv \mathcal{V}\left(\Lambda_i, n_i, \frac{m_i 2^{m(n_i)\nu}}{n_i} \hat{J} + \sum_{j=0}^{m(n_i)-1} \left(\frac{C_{ij} 2^{j\nu}}{n_i}\right) \tilde{J}\right) \\ &\geq [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(\xi^\nu v'), 2^{m(n_i)\nu}, \hat{J}^{\Delta_i})]^{m_i} \\ &\quad \times \prod_{j=0}^{m(n_i)-1} [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(\xi^\nu v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}})]^{C_{ij}}, \end{aligned}$$

where $\Delta_i = \Delta n_i / \theta_{\kappa''}^{\lambda m(n_i)} R_0^\lambda$.

A short computation gives $\Delta_i < C \Delta_{\kappa'' - \kappa', m(n_i)}$ for $C = 2^{\kappa'(\lambda - \nu)} \varphi_{\kappa'' - \kappa'}^{-1}$, and $\Delta_{\kappa, j} \geq A \varphi_{\kappa} 2^{\nu + \kappa(\lambda - \nu)} / R_0^\lambda 2^{\kappa(\lambda - \nu) m(n_i)}$ for $0 \leq j < m(n_i)$. Hence, for large enough i , $\Delta_i < \Delta_{\kappa, j}$, so that $\tilde{J}^{\Delta_{\kappa, j}} \subset \tilde{J}^{\Delta_i}$. Similarly, it is seen that $\Lambda_{\kappa, j}(v') \subset \Lambda_{\kappa'', m(n_i)}(\xi^\nu v')$ and $\Lambda_{\kappa'', m(n_i)}(v') \subset \Lambda_{\kappa'', m(n_i)}(\xi^\nu v')$. Writing $N_1 = \inf\{m \in \mathbb{Z}_+ \mid \Lambda_{\kappa, m}(v') \neq \emptyset\} \in \{0, 1, \dots, m(n_i) - 1\}$, we obtain

$$\mathcal{V}_i \geq [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(v'), 2^{m(n_i)\nu}, \hat{J}^{C \Delta_{\kappa'' - \kappa', m(n_i)}})]^{m_i}$$

$$\times \prod_{j=0}^{N_1-1} [\mathcal{V}(\Lambda_{\kappa, N_1}(v'), 2^{j\nu}, J^{\Delta_{\kappa, j}})]^{C_{ij}}$$

$$\times \prod_{j=N_1}^{m(n_i)-1} [\mathcal{V}(\Lambda_{\kappa, j}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}})]^{C_{ij}}.$$

Next $\tilde{J} \in \mathcal{C}_t$ will be fixed to guarantee that each of the factors above will be nonzero. Choose $x_0 \in \mathbb{R}^t$ such that $s_\kappa(v', x_0) > -\infty$ and let $J_{-1} \in \mathcal{C}_t$ be a rectangular solid with edges $\{(a_{-1k}, b_{-1k})\}_{k=1}^t$ containing x_0 . Then, for all $j \geq N_2$, $\mathcal{V}(\Lambda_{\kappa, j}(v'), 2^{j\nu}, J_{-1}^{\Delta_{\kappa, j}}) > 0$, where $N_2 = \inf\{j \in \mathbb{Z}_+ \mid \mathcal{V}(\Lambda_{\kappa, j}(v'), 2^{j\nu}, J_{-1}^{\Delta_{\kappa, j}}) > 0\}$, and, for i large, $0 \leq N_2 < m(n_i)$. Let $J_j \in \mathcal{C}_t$ be a rectangular solid with edges $\{(a_{jk}, b_{jk})\}_{k=1}^t$ such that $\mathcal{V}(\Lambda_{\kappa, N_1}(v'), 2^{j\nu}, J_j^{\Delta_{\kappa, j}}) > 0$ for $0 \leq j < N_1$, and $\mathcal{V}(\Lambda_{\kappa, j}(v'), 2^{j\nu}, J_j^{\Delta_{\kappa, j}}) > 0$ for $N_1 \leq j < N_2$. Then define J to be a rectangle with sides $\{(a_k, b_k)\}_{k=1}^t$, where

$$a_k = \left(\inf_{-1 \leq j < N_3} a_{jk}\right) - \Delta_{\kappa,0}, \quad b_k = \left(\inf_{-1 \leq j < N_3} b_{jk}\right) + \Delta_{\kappa,0},$$

$$N_3 = \sup\{N_1, N_2\}.$$

Since

$$\lim_{i \rightarrow \infty} \sum_{j=0}^{m(n_i)-1} \frac{C_{ij} 2^{j\nu}}{n_i} = 0 \quad \text{and} \quad \lim_{i \rightarrow \infty} \frac{m_i 2^{m(n_i)\nu}}{n_i} = 1,$$

for i large enough,

$$\frac{m_i 2^{m(n_i)\nu}}{n_i} \hat{J} + \sum_{j=0}^{m(n_i)-1} \left(\frac{C_{ij} 2^{j\nu}}{n_i} \right) \tilde{J} \subset J^{d_i}.$$

Using this and 2.3(iii),

$$\liminf_{i \rightarrow \infty} \frac{1}{n_i} \log V(\Lambda_i, n_i, J^{d_i}) \geq S_{\kappa}(v', \tilde{J}) + \liminf_{i \rightarrow \infty} \sigma_i$$

for

$$\begin{aligned} |\sigma_i| &= \frac{1}{n_i} \left| \sum_{j=0}^{N_1-1} C_{ij} 2^{j\nu} \frac{1}{2^{j\nu}} \log V(\Lambda_{\kappa, N_1}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}}) \right. \\ &\quad \left. + \sum_{j=N_1}^{m(n_i)-1} C_{ij} 2^{j\nu} \frac{1}{2^{j\nu}} \log V(\Lambda_{\kappa, j}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}}) \right| \\ &\leq \frac{m(n_i) 2^{m(n_i)\nu}}{n_i} \sup \left\{ \sup_{0 \leq j < N_1} \left| \frac{1}{2^{j\nu}} \log V(\Lambda_{\kappa, N_1}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}}) \right| \right. \\ &\quad \left. \sup_{N_1 \leq j < m(n_i)} \left| \frac{1}{2^{j\nu}} \log V(\Lambda_{\kappa, j}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa, j}}) \right| \right\}. \end{aligned}$$

But the first term in the supremum is finite by construction of \tilde{J} and nondependence of N_1 on i , and the second term is equal to

$$\begin{aligned} \sup \left\{ \frac{1}{2^{N_1\nu}} \left| \log V(\Lambda_{\kappa, N_1}(v'), 2^{N_1\nu}, \tilde{J}^{\Delta_{\kappa, N_1}}) \right| \right. \\ \left. \frac{1}{2^{(m(n_i)-1)\nu}} \left| \log V(\Lambda_{\kappa, m(n_i)-1}(v'), 2^{(m(n_i)-1)\nu}, \tilde{J}^{\Delta_{\kappa, m(n_i)-1}}) \right| \right\}. \end{aligned}$$

Here again the first term is finite by choice of \tilde{J} , and the second term is bounded by $2 + \log v'$, hence $\lim_{i \rightarrow \infty} |\sigma_i| = 0$.

Lemma 3.4¹: If $\{\Lambda_i\}_{i=1}^{\infty} \subset \mathcal{C}$, each Λ_i is connected, and $\Lambda_i \rightarrow \infty$ (Fisher), then $\inf_i V(\Lambda_i)/V(\tilde{\Lambda}_i) > 0$, where $\tilde{\Lambda}_i$ is any minimal cube containing Λ_i .

Theorem 3.5: Suppose $\{(\Lambda_i, n_i)\}_{i=1}^{\infty}$ is a Fisher system tending to density $1/v$, each Λ_i is connected, $\kappa \in (0, \kappa)$, $J \in \tilde{\mathcal{C}}_t(v)$, and $S_{\kappa}(v, J) > -\infty$. Then there exists a decreasing sequence $\{d_i\}_{i=1}^{\infty}$ of strictly positive real numbers converging to zero, such that

$$S_{\kappa, 0}(v, J) \geq \limsup_{i \rightarrow \infty} \frac{1}{n_i} \log V(\Lambda_i, n_i, J^{d_i}).$$

Proof: For $i \in \mathbb{Z}_+$, let $p(i) = 1 + \inf\{m \in \mathbb{Z}_+ \mid \Lambda_{\kappa, m}(v) \text{ contains a translate } \Lambda'_i \text{ of } \Lambda_i\}$, so that $\Lambda_{\kappa, p(i)-1}(v)$ is the minimal standard cube containing Λ_i . Writing $d_i = A \varphi_{\kappa} 2^{p(i)\nu} / \theta_{\kappa}^{\lambda p(i)} R_{\kappa}$, if $\tilde{\Lambda}_i$ is any minimal cube containing Λ_i , then

$$2^{\nu} \leq V(\Lambda_{\kappa, p(i)}(v)) / V(\tilde{\Lambda}_i) \leq (2^{\nu} + 1)^2$$

for i sufficiently large, so

$$\frac{1}{2^{\nu}} \geq \frac{V(\Lambda_i)}{V(\Lambda_{\kappa, p(i)}(v))} > \frac{1}{(2^{\nu} + 1)^2} \inf_i \frac{V(\Lambda_i)}{V(\tilde{\Lambda}_i)} > 0.$$

Now pass to a subsequence $\{\Lambda_{i_j}\}_{j=1}^{\infty}$ such that

$$\lim_{j \rightarrow \infty} \frac{V(\Lambda_{i_j})}{V(\Lambda_{\kappa, p(i_j)}(v))} = \beta$$

and

$$\lim_{j \rightarrow \infty} \frac{1}{n_{i_j}} \log V(\Lambda_{i_j}, n_{i_j}, J^{d_{i_j}}) = \limsup_{i \rightarrow \infty} \frac{1}{n_i} \log V(\Lambda_i, n_i, J^{d_i}).$$

Let $\Lambda_i'' = \{q \in \Lambda_{\kappa, p(i)}(v) / \Lambda'_i \mid d(q, \Lambda'_i) > \theta_{\kappa}^{p(i)} R_{\kappa}\}$ and $n_i'' = 2^{p(i)\nu} - n_{i_j}$. It can be shown, as in Ref. 1, that $\Lambda_i'' \rightarrow \infty$ (Fisher) and it is easy to see that $\lim_{j \rightarrow \infty} V(\Lambda_{i_j}'') / V(\Lambda_{\kappa, p(i_j)}(v)) = 1 - \beta$. By computing $\lim_{j \rightarrow \infty} n_i'' / 2^{p(i)\nu} = 1 - \beta$, therefore $\lim_{j \rightarrow \infty} V(\Lambda_{i_j}'') / n_i'' = v$. Since Λ_{i_j}' and Λ_{i_j}'' may be translated inside $\Lambda_{\kappa, p(i_j)}(v)$ with mutual separation $\theta_{\kappa}^{p(i_j)} R_{\kappa} \geq R_0$, for large enough j ,

$$\begin{aligned} \frac{1}{2^{p(i_j)\nu}} \log V(\Lambda_{\kappa, p(i_j)}(v), 2^{p(i_j)\nu}, J) \\ \geq \frac{n_{i_j}}{2^{p(i_j)\nu}} \frac{1}{n_{i_j}} \log V(\Lambda_{i_j}, n_{i_j}, J^{d_{i_j}}) \\ + \frac{n_i''}{2^{p(i_j)\nu}} \frac{1}{n_i''} \log V(\Lambda_{i_j}'', n_i'', J^{d_{i_j}}). \end{aligned}$$

The theorem follows from 3.3.

Corollary 3.6: Suppose $\{(\Lambda_i, n_i)\}_{i=1}^{\infty}$ is a Fisher system tending to density $1/v$, $v \neq v_0$, with each Λ_i connected, and f is an asymptotically open t -valued observable with $\lambda > v$. Then, if $J \in \tilde{\mathcal{C}}_t(v)$,

$$\lim_{i \rightarrow \infty} \frac{1}{n_i} \log V(\Lambda_i, n_i, J) = S(v, J)$$

exists, and

$$s(v, x) = \inf_{x \in J \in \tilde{\mathcal{C}}_t} S(v, J)$$

is given by

$$s(v, x) = s_{\kappa, 0}(v, x), \quad \kappa \in (0, \kappa).$$

Therefore, s has the continuity and concavity properties of Corollaries 1.7 and 1.10.

The existence of the limit follows from 3.3 and 3.5 by removal of the contractions from J^{d_i} as in 2.3, and from an argument similar to 3.5.

We note that when $t=1$ and f is the potential energy U of a tempered interaction, $s(v, \epsilon)$ is the usual microcanonical configurational entropy per particle for a system at density $1/v$ and interaction energy per particle ϵ .

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