NONEQUILIBRIUM STATISTICAL MECHANICS AND ENTROPY PRODUCTION IN A CLASSICAL INFINITE SYSTEM OF ROTATORS.

by David Ruelle*.

Abstract. *We analyze the dynamics of a simple but nontrivial classical Hamiltonian system of infinitely many coupled rotators. We assume that this infinite system is driven out of thermal equilibrium either because energy is injected by an external force (Case I) , or because heat flows between two thermostats at different temperatures (Case II). We discuss several possible definitions of the entropy production associated with a finite or infinite region, or with a partition of the system into a finite number of pieces. We show that these definitions satisfy the expected bounds in terms of thermostat temperatures and energy flow.*

Keywords: nonequilibrium statistical mechanics, entropy production, phase space volume contraction, rotators.

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0 Introduction.

In the present paper, we study certain classical Hamiltonian systems consisting of an infinite number of coupled degrees of freedom (rotators or "little wheels"). For a system in the class considered, the time evolution (f^t) is well defined, and given by the limit (in some sense) of the Hamiltonian time evolution for finite subsystems. [Note that other infinite systems, like gases of interacting particles, would be much more difficult to control]. A probability measure on the phase space of the infinite system is called a *state*, and it has a well-defined time evolution. We introduce a family of initial states called Γ-states (they are Gibbs states of some sort). Some of these Γ-states describe a situation where parts of our infinite system (thermostats) are at given temperatures. For a Γ-state ℓ, the time-evolved state $f^t\ell$ gives a finite Gibbs entropy $S^t(X)$ to each finite subsystem X of the infinite system L. If X is infinite (but has finite interaction with the rest of the system) the difference $\Delta S^t(X) = \lim_{Y\to\infty}(S^t(X\cap Y) - S^0(X\cap Y))$ still makes sense.

The bulk of the paper is dedicated to a discussion of the (nontrivial) dynamics of our infinite system of rotators. Understanding the dynamics of the system is a necessary prerequisite to analyzing its nonequilibrium statistical mechanics. We shall in fact examine a specific nonequilibrium problem: is it possible to define a local rate of entropy production (associated with a finite region X) in a nontrivial manner? This possibility has been suggested by Denis Evans and coworkers [16]. We examine their proposal and some alternatives, but obtain only partial results. Because of the obvious physical interest of the problem, we now give some details.

By time-averaging $f^t\ell$ or $d\Delta S^t(X)/dt$ (over a suitable sequence of intervals $[0,T]\to\infty$) we may define a nonequilibrium steady state

$$\rho = \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, f^t\ell$$

and an average rate of entropy growth

$$\sigma(X) = \lim_{T\to\infty}\frac{1}{T}\Delta S^T(X)$$

(we do not know that $\sigma(X)$ is uniquely determined by ρ and X).

We ask if an entropy production rate $e(X)$ can be meaningfully associated with a finite set $X\subset L$. For definiteness we shall think of two physical situations. In Case I there is a finite set X_0 such that an external force acts on X_0, and the initial state ℓ restricted to $L\backslash X_0$ corresponds to thermal equilibrium at temperature β^{-1}. In Case II we have $L = X_0 \sqcup L_1 \sqcup L_2$ where X_0 is finite, L_1 and L_2 are infinite and ℓ restricted to L_i corresponds to thermal equilibrium at temperature β_i^{-1} (with $\beta_1^{-1} < \beta_2^{-1}$). There is a thermodynamic formula for the global rate of entropy production:

$$e_\Theta = \beta \times \text{energy flux to thermostat} \qquad \text{(Case I)}$$

$$e_\Theta = (\beta_1 - \beta_2) \times \text{energy flux to thermostat 1} \qquad \text{(Case II)}$$

[Note that Case I resembles Case II, where thermostat 2 is replaced by the external force, and ascribed an infinite temperature ($\beta_2 = 0$)]. The question is how to define a local rate of entropy production $e(X) \geq 0$ such that $\sup_{X \text{ finite}} e(X) = e_\Theta$.

The original proposal by Evans and coworkers* is to take, for X finite,

$$e(X) = -\sigma(X)$$

This is shown to be the average rate of volume contraction in the phase space $[X]$ of the subsystem X due to the fluctuating forces to which it is subjected by the complementary subsystem $L\backslash X$.

Another idea is to replace the entropy $S(X)$ by the conditional entropy given formally by $\check{S}(X) = S(L) - S(L\backslash X)$. The corresponding rate of entropy production is

$$\check{e}(X) = \sigma(L\backslash X)$$

We shall make the important physical assumption that the expectation value of the energy for each finite system X has a bound independent of time**. It follows that $\check{e}(X)$ is finite, and one has

$$0 \leq e(X) \leq \check{e}(X)$$

Instead of using a finite set X one may base a definition of entropy production rate on a finite partition $\mathcal{A} = (X_0, X_1, \ldots, X_n)$ of L, with finite boundary (this will be made precise later). We define

$$e(\mathcal{A}) = \sum_{j=0}^{n} \sigma(X_j) \qquad , \qquad \check{e}(\mathcal{A}) = \sum_{j:X_j \text{ infinite}} \sigma(X_j)$$

In particular, in Case II, for X finite $\supset X_0$, we have

$$\check{e}(X) = \check{e}((X, L\backslash X)) \leq \check{e}((X, L_1\backslash X, L_2\backslash X))$$

and the right-hand side $e((X, L_1\backslash X, L_2\backslash X))$ seems a rather natural definition of entropy production rate.

We shall later study further properties of the entropy production rates defined above, but we note here that they are all bounded by the thermodynamic expression e_Θ. The

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* Actually, the ideas presented in [16] are formulated for Case I, and for a system thermostatted at the boundary rather than an actually infinite system. While the two idealizations are technically quite different, they are expected to give the same results in cases of physical interest.

** Note that in Case I, if the system has dimension ≤ 2, the external force may cause an infinite accumulation of energy in a finite region. Our assumption that the nonequilibrium steady state ρ gives a finite expectation to the energy of finite subsystems is thus invalid, and so is our analysis.

problem is to prove that they depend effectively on X or $\mathcal{A}$, and are not identically equal to 0 or e_Θ.

We now recall some earlier work to put the problem of defining a local entropy production rate in perspective.

In earlier studies of quantum spin systems [15], [11], the global entropy production (for Case II) was defined by the thermodynamic relation

$$e_\Theta = (\beta_1 - \beta_2) \times \text{energy flux to thermostat 1}$$

but the quantities $e(X)$, $\check{e}(X)$ were not introduced because they would automatically vanish. This is because, for quantum spin systems we have $|\check{S}^t(X)| < S^t(X)$ (see [3] Proposition 6.2.28(b)); for classical rotators by contrast, the entropy is not bounded below.

The statistical mechanics of classical systems outside of equilibrium can be studied in models with nongradient forces and a "deterministic thermostat" [7], [10]. Such a nonhamiltonian system corresponds in effect to a rather general time evolution (f^t) defined by a vector field $\mathcal{X}$ on a finite dimensional manifold M. In general, no absolutely continuous invariant measure (*i.e.*, "phase space volume" m) on M is preserved by the time evolution, but one may assume that there is a natural (singular) measure ρ describing a nonequilibrium steady state. One can argue that the average phase space volume contraction $\int \rho(dx)(-\mathrm{div}_m \mathcal{X})(x)$ is the rate of entropy production by the system. This identification (for which see Andrei [1]) has been used in particular by Evans, Cohen, and Morriss [6], and by Gallavotti and Cohen [9] in the study of fluctuations of the entropy production. See also the work of Posch and Hoover [13], Gallavotti [8].

Note now that if we introduce a nongradient force $\xi(q)$ in the Hamiltonian equations of motion, the volume $dp\,dq$ is preserved, but energy conservation is lost and this is why a thermostat is needed. In the case of a deterministic thermostat, the phase space contraction is caused by the thermostat (as one can check in the example of the *isokinetic thermostat* corresponding to an added "force" $-\alpha(p,q)p$, where $\alpha(p,q) = p \cdot \xi(q)/p \cdot p$). In the lab however the thermostat is of a different nature: it is typically a large system (reservoir) with which the small system of interest can exchange heat, and it is not clear at first how to define entropy production. In particular, a nonequilibrium steady state for the infinite system L may well have absolutely continuous projection on the phase space of the small system X [4], [5], [2], which contradicts $e(X) > 0$ but may allow $\check{e}(X) > 0$.

Finally, to indicate the difficulty of the problems considered here, and in particular of proving $\check{e}(X) > 0$, consider Case II in dimension ≤ 2. There (as indicated by the macroscopic continuous limit), $f^t\ell$ presumably tends to an *equilibrium* state ρ and the entropy production $\check{e}(X)$ vanishes for all X.

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1 Description of the model.

Our system will be an infinite collection of rotators labelled by $x \in L$, each with Hamiltonian $H_x(p_x, q_x) = p_x^2/2 + V_x(q_x)$, where $p_x \in \mathbf{R}$, $q_x \in \mathbf{T}$. [This is for simplicity; it would probably be easy to replace the rotators by more complicated systems]. We let Γ be a set of unordered pairs $\{x, y\}$ of points in L, *i.e.*, Γ is a graph with vertex set L, and we define a formal Hamiltonian for the infinite system of little wheels:

$$\sum_{x \in L} H_x(p_x, q_x) + \sum_{\{x,y\} \in \Gamma} W_{\{x,y\}}(q_x, q_y)$$

The functions V_x, $W_{\{x,y\}}$ are assumed to be smooth.

For $X \subset L$, let $\Gamma_X = \{\{x, y\} \in \Gamma : x, y \in X\}$ and, when X is finite, write

$$H_X(p_X, q_X) = \sum_{x \in X} H_x(p_x, q_x) + \sum_{\{x,y\} \in \Gamma_X} W_{\{x,y\}}(q_x, q_y)$$

where $p_X = (p_x)_{x \in X} \in \mathbf{R}^X$, $q_X = (q_x)_{x \in X} \in \mathbf{T}^X$. We shall also make use of a constant external force* $F \in \mathbf{R}^{X_0}$ acting on a finite set X_0.

For finite X, a time evolution (f_X^t) on $\mathbf{R}^X \times \mathbf{T}^X$ is defined by

$$\frac{d}{dt} \begin{pmatrix} p_X \\ q_X \end{pmatrix} = \begin{pmatrix} F_X - \partial_{q_X} H_X(p_X, q_X) \\ p_X \end{pmatrix}$$

where the term F_X is the component of F in $\mathbf{R}^X$, and is present only in case I. We have thus

$$f_X^t(p_X(0), q_X(0)) = (p_X(t), q_X(t))$$

We shall suppose that Γ is connected and, for $x, y \in L$, define

$$d(x, y) = \min\{k : \exists x_0, \ldots, x_k \in L \text{ with } x_0 = x, x_k = y \text{ and } \{x_{j-1}, x_j\} \in \Gamma \text{ for } j = 1, \ldots k\}$$

We write then $B_x^k = \{y : d(x, y) \leq k\}$.

1.1 Assumption (finite dimensionality).
There is a polynomial $P(k)$ such that for all $x \in L$ and $k \geq 0$

$$|B_x^k| \leq P(k)$$

[We may take $P(k) = 1 + ak^b$ for some $a, b > 0$; Γ is thus assumed to have order $\leq a$, and "dimension" $\leq b$].

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* F is taken constant for simplicity. More generally one could consider the case of a smooth function $F(q_{X_0}, \phi^t\alpha)$ of q_{X_0} and $\phi^t\alpha$ with values in $\mathbf{R}^{X_0}$, where (ϕ^t) is a smooth dynamical system on a compact manifold $\mathcal{A}$, and α is distributed according to some prescribed (ϕ^t)-ergodic measure on $\mathcal{A}$.

Note that by compactness of $\mathbf{T}$ and the assumed smoothness of V_x, $W_{\{x,y\}}$, every "force" term (*i.e.*, each component F_x of F for $x \in X_0$, each $\partial_{q_x} V_x$, each $\partial_{q_x} W_{\{x,y\}}$, $\partial_{q_y} W_{\{x,y\}}$) is bounded, and has bounded derivatives with respect to its arguments q_z.

1.2 Assumption (uniform boundedness).

The force terms $\partial_{q_x} V_x$, $\partial_{q_x} W_{\{x,y\}}$, $\partial_{q_y} W_{\{x,y\}}$ and their q_z-derivatives (up to any finite order) are bounded uniformly in $x, y \in L$.

1.3 Lemma (uniform boundedness of forces).

The forces $F_x - \partial_{q_x} H_X(p_X, q_X)$ or $-\partial_{q_x} H_X(p_X, q_X)$ and their q_z-derivatives have modulus bounded respectively by constants K, K'. [We shall also denote by $\bar{K}$ a constant $\geq 2K, P(1)K', 1$].

This follows from Assumptions 1.1 and 1.2 [only the bounded order of Γ is used from Assumption 1.1]. □

2 Time evolution of infinite systems.

For $X \subset L$, we shall from now on write $[X] = (\mathbf{R} \times \mathbf{T})^X$. We note the following facts which follow from Lemma 1.3.

(i) For X finite and $\xi \in [X]$, if $f_X^t \xi = (p_x(t), q_x(t))_{x \in X}$ we have the estimate

$$|p_x(t) - p_x(0)| \leq K|t| \quad \text{when} \quad x \in X$$

(ii) For $\tilde{X}$ finite and $\tilde{\xi} \in [\tilde{X}]$ let also $f_{\tilde{X}}^t \tilde{\xi} = (\tilde{p}_x(t), \tilde{q}_x(t))_{x \in \tilde{X}}$. Then, if $p_x(0) = \tilde{p}_x(0)$, $q_x(0) = \tilde{q}_x(0)$ for some $x \in X \cap \tilde{X}$ we have

$$|p_x(t) - \tilde{p}_x(t)| \leq 2K|t|$$

$$|q_x(t) - \tilde{q}_x(t)| \leq K|t|^2$$

and since $|q_x(t) - \tilde{q}_x(t)| \leq 1 \leq \bar{K}$, we also have

$$|q_x(t) - \tilde{q}_x(t)| \leq [K|t|^2 . \bar{K}]^{\frac{1}{2}} \leq \bar{K}|t|$$

so that

$$\max(|p_x(t) - \tilde{p}_x(t)|, |q_x(t) - \tilde{q}_x(t)|) \leq \bar{K}|t|$$

(iii) Let $k \geq 0$ and $X \supset B_x^k$, $\tilde{X} \supset B_x^k$. Then, with the notation of (ii), if

$$(\forall y \in B_x^k) \qquad p_y(0) = \tilde{p}_y(0) \quad \text{and} \quad q_y(0) = \tilde{q}_y(0)$$

we have

$$\max(|p_x(t) - \tilde{p}_x(t)|, |q_x(t) - \tilde{q}_x(t)|) \leq \frac{(\bar{K}|t|)^{k+1}}{(k+1)!}$$

indeed, by the equation of motion and induction on k we have

$$|\frac{d}{dt}(f_X^t \xi - f_X^t \tilde{\xi})| \leq \bar{K} \frac{(\bar{K}|t|)^k}{k!}$$

and the desired result follows by integration.

2.1 Lemma (a priori estimates).

For finite $X, \tilde{X} \subset L$, *let* $\xi \in [X]$, $\tilde{\xi} \in [\tilde{X}]$, *and* $f^t_X\xi = (\xi_x(t))_{x\in X} = (p_x(t), q_x(t))$, $f^t_{\tilde{X}}\tilde{\xi} = (\tilde{\xi}_x(t))_{x\in\tilde{X}} = (\tilde{p}_x(t), \tilde{q}_x(t))$. *With this notation,*
(a) $\quad |p_x(t) - p_x(0)| \leq K|t|$, *hence* $|p_x(t)| \leq |p_x(0)| + K|t|$
(b) if $k > 0$, *and* $B^{k-1}_x \subset X \cup \tilde{X}$, *and* $\xi_y(0) = \tilde{\xi}_y(0)$ *for all* $y \in B^{k-1}_x$, *then*

$$|\xi_x(t) - \tilde{\xi}_x(t)| = \max[|p_x(t) - \tilde{p}_x(t)|, |q_x(t) - \tilde{q}_x(t)|] \leq \frac{(\bar{K}|t|)^k}{k!}$$

This follows from (i) and (iii) above [(b) is a rather rough estimate, but sufficient for our purposes]. ∎

2.2 Proposition (time evolution).

Let $(p_x(0), q_x(0))_{x\in L} \in [L]$ *be given. For finite* $X \subset L$, *write* $(p^X_x(t), q^X_x(t))_{x\in X} = f^t_X(p^X_x(0), q^X_x(0))_{x\in X}$. *Then for each* $x \in L$ *the limits*

$$\lim_{d(x,L\backslash X)\to\infty} p^X_x(t) = p_x(t) \qquad , \qquad \lim_{d(x,L\backslash X)\to\infty} q^X_x(t) = q_x(t)$$

exist, and $(p_x(t), q_x(t))_{x\in L}$ *is the unique solution of the infinite system evolution equation with initial condition* $(p_x(0), q_x(0))_{x\in L}$. *We write* $(p_x(t), q_x(t))_{x\in L} = f^t(p_x(0), q_x(0))_{x\in L}$.

The existence of the limit follows from Lemma 2.1. Writing the infinite system evolution equation is left to the reader, as well as checking that $(p_x(t), q_x(t))_{x\in L}$ is the unique solution. ∎

2.3 Remarks.

The limits in Proposition 2.2 are faster than $\exp(-k\, d(x, L\backslash X))$ for any $k > 0$, independently of $(p_x(0), q_x(0))_{x\in L}$, and uniformly for t in any compact interval $[-T, T]$.

Existence and uniqueness theorems are known in more difficult situations; see for instance [12].

The proof of Proposition 2.2 does not use the finite dimensionality of Γ, only its finite order.

2.4 Notation.

In principle we use the notation $(p^X_x(t), q^X_x(t))_{x\in X}$ for the finite system time evolution (f^t_X), and $(p_x(t), q_x(t))_{x\in L}$ for the infinite system evolution (f^t), but it will often be convenient to drop the superscript X.

It is useful to compactify the momentum space $\mathbf{R}$ to a circle $\dot{\mathbf{R}}$ by addition of a point at infinity for each $x \in L$, and write $[\dot{X}] = (\dot{\mathbf{R}} \times \mathbf{T})^X$ for $X \subset L$. The phase space of our infinite system is then $[L] = (\mathbf{R} \times \mathbf{T})^L \subset (\dot{\mathbf{R}} \times \mathbf{T})^L = [\dot{L}]$. We shall use the product topologies on $[L] = (\mathbf{R} \times \mathbf{T})^L$ and $[\dot{L}] = (\dot{\mathbf{R}} \times \mathbf{T})^L$; therefore $[\dot{L}]$ is compact and $[L]$ has the topology it inherits as subset of $[\dot{L}]$. If $U \subset L$ we denote by π_U the projection

$$\pi_U : [\dot{L}] = [\dot{U}] \times [\dot{L\backslash U}] \to [\dot{U}]$$

2.5 Proposition (continuity of f^t).

The map $(\xi, t) \mapsto f^t\xi$ is continuous $[L] \times \mathbf{R} \to [L]$ and, for each t, $f^t : [L] \to [L]$ is a homeomorphism.

To prove the continuity of $(\xi, t) \mapsto f^t\xi$, it suffices to prove the continuity of $(\xi, t) \mapsto (p_x(t), q_x(t))$ for each $x \in L$, and this results from the uniformity of the limits in Proposition 2.2 (see Remark 2.3). By uniqueness of f^t, the map f^{-t} is the inverse of f^t and, since $f^{-t} : [L] \to [L]$ is continuous, f^t is a homeomorphism. $\square$

2.6 Proposition (smoothness of f^t).

Let $X \subset Y$, X finite and Y finite or $= L$. For $\xi \in [X]$, $\eta \in [Y\backslash X]$, write $f^t_Y(\xi, \eta) = (p_x(t), q_x(t))_{x\in Y}$. Then, for fixed η and each $x \in Y$, the map $(\xi, t) \mapsto (p_x(t), q_x(t))$ is smooth $[X] \times \mathbf{R} \to \mathbf{R} \times \mathbf{T}$.

This results from the bounds on the derivatives (uniform in Y) obtained in Proposition 2.7 below.

2.7 Proposition (estimate of derivatives).

Let $Y \subset L$, Y finite or $= L$, and

$$f^t_Y(\eta_x(0))_{x\in Y} = (\eta_x(t))_{x\in Y} = (p_x(t), q_x(t))$$

Write

$$r^{(i,j)}_x(t; x_1, \ldots, x_j) = \frac{\partial^i}{\partial t^i}\frac{\partial}{\partial\eta_{x_1(0)}}\cdots\frac{\partial}{\partial\eta_{x_j(0)}}\eta_x(t)$$

where $x_1, \ldots, x_j$ need not be all distinct; then

$$|r^{(i,j)}_x(t; x_1, \ldots, x_j)| \le \mathcal{P}_{ij}((|p_y(0)| + K|t|))$$

where $\mathcal{P}_{ij}((p_y))$ is a polynomial of degree $\le i+1$ (the degree is 1 if $(i,j) = (0,0)$, $\le i$ otherwise) in the p_y with $y \in B^i_x$.

Let $\sigma = \sigma(x, x_1, \ldots, x_j)$ denote the smallest number of edges of a connected subgraph of Γ having $x, x_1, \ldots, x_j$ among its vertices. Then the coefficients of $\mathcal{P}_{ij}$ are positive and

$$\le M_{ij}e^{j\bar{K}|t|}\frac{(L_j|t|)^\tau}{\tau!}$$

with suitable $L_j, M_{ij} > 0$, for all τ such that $0 \le \tau \le [\sigma - i]_+$ where we have written $[\sigma - i]_+ = \max(0, \sigma - i)$.

The proof is given in Appendix A.1.

2.8 Proposition (estimate of differences).

We use the notation of Proposition 2.7. Let $(\eta_x(0)), (\tilde{\eta}_x(0)) \in [Y]$ *and define* $\tilde{r}_x^{(i,j)}$ *as* $r_x^{(i,j)}$ *with* η *replaced by* $\tilde{\eta}$. *For finite* $X \subset L$ *we assume* $\eta_y(0) = \tilde{\eta}_y(0)$ *when* $y \notin X$, *and write*

$$\Delta r_x^{(i,j)}(t; x_1, \ldots, x_j; X) = r_x^{(i,j)}(t; x_1, \ldots, x_j; X) - \tilde{r}_x^{(i,j)}(t; x_1, \ldots, x_j; X)$$

If $d(x, X) > i$, *we have*

$$|\Delta r_x^{(i,j)}(t; x_1, \ldots, x_j; X)| \leq \mathcal{Q}((|p_y(0)| + K|t|))$$

where $\mathcal{Q}((p_y))$ *is a polynomial of degree* $\leq i+1$ *(the degree is* 1 *if* $(i,j) = (0,0)$, $\leq i$ *otherwise) in the* p_y *with* $y \in B_x^i$.

Let $\sigma = \sigma(x, x_1, \ldots, x_j; X)$ *denote the smallest number of edges of a subgraph of* Γ *(not necessarily connected) connecting each point* $x, x_1, \ldots, x_j$ *to some point of* X. *Then the coefficients of* $\mathcal{Q}_{ij}$ *are positive and*

$$\leq M_{ij} e^{j\bar{K}|t|} \frac{(L_j|t|)^\tau}{\tau!}$$

for all τ *such that* $0 \leq \tau \leq \sigma - i$

The proof is given in Appendix A.2.

2.9 Remarks

Proposition 2.7, 2.8 will be used in the proof of Theorem 4.5 below. In view of these applications the following facts should be noted.

(a) The condition $d(x, X) > i$ in Proposition 2.8 is not a serious limitation because, for the finitely many values of x such that $d(x, X) \leq i$, one can estimate $\Delta r^{(i,j)}$ by Proposition 2.7 applied to $r^{(i,j)}$ and $\tilde{r}^{(i,j)}$.

(b) Write $\sigma = \sigma(y, y_1, \ldots, y_j)$ and let y be fixed, then

$$\sum_{y_1, \ldots, y_j} \frac{1}{(\sigma - i)!} < \infty$$

Indeed, we have $|y_k - y| \leq \sigma$, hence

$$\sigma - i \geq \sum_{k=1}^{j} \frac{|y_k - y| - i}{j}$$

so that $1/(\sigma - i)!$ decreases faster than exponentially with respect to $r_1 = |y_1 - y|, \ldots, r_j = |y_j - y|$, while $|B_y^{r_1}| \cdots |B_y^{r_j}|$ is polynomially bounded.

3 Time evolution for probability measures.

Consider any probability measure ℓ on $[\dot{L}] = (\dot{\mathbf{R}} \times \mathbf{T})^L$ carried by $[L] = (\mathbf{R} \times \mathbf{T})^L$ (*i.e.*, ℓ gives zero measure to the points at infinity). We can find constants $\kappa_{nx} > 0$ such that, if we write

$$B_n = \{(p_x, q_x)_{x\in L} : |p_x| \le \kappa_{nx} \text{ for all } x \in L\}$$

we have $\ell(B_n) > 1 - 1/n$. We may thus write $\lim_{n\to\infty} ||\ell - \ell_n|| = 0$ where the measure ℓ_n has support in the compact set $B_n \subset [L]$, and $(t, \xi) \to f^t\xi$ is continuous on $\mathbf{R} \times B_n$. We define then

$$f^t\ell = \lim_{n\to\infty} f^t\ell_n \qquad \text{(norm limit)}$$

Notice also that $f^t\ell_n$ has support in the compact set B'_n defined like B_n with κ_{nx} replaced by $\kappa'_{nx} = \kappa_{nx} + K|t|$ (see Lemma 2.1(a)). Therefore $f^t\ell$ is again carried by $[L]$.

3.1 Proposition (continuity of time evolution).

If the probability measure ℓ on $[\dot{L}]$ is carried by $[L]$, then the probability measure $f^t\ell$ is well defined, carried by $[L]$, and $t \mapsto f^t\ell$ is continuous $\mathbf{R} \to$ measures on $[\dot{L}]$ with the vague topology.

For any continuous function $A : [\dot{L}] \to \mathbf{R}$ we have $(f^t\ell_n)(A) = \ell_n(A \circ f^t)$, where $A \circ f^t$ restricted to B_n depends continuously on t with respect to the uniform norm on $\mathcal{C}(B_n \to \mathbf{R})$. Therefore $(f^t\ell_n)(A)$ is a continuous function of t, and so is its uniform limit $t \mapsto f^t\ell(A)$. This shows that $t \mapsto f^t\ell$ is continuous with respect to the w^* (=vague) topology of measures on $[\dot{L}]$, concluding the proof. ∎

Let ℓ_X be a probability measure on $[\dot{X}]$ for finite $X \subset L$. We write $X \to \infty$ when, for every finite $U \subset L$, eventually $X \supset U$. Suppose that for every finite U and $A \in \mathcal{C}([\dot{U}] \to \mathbf{R})$ the limit

$$\lim_{X\to\infty} \ell_X(A \circ \pi_{UX})$$

exists, where π_{UX} is the projection $[\dot{X}] = [X \dot{\backslash} U] \times [\dot{U}] \to [\dot{U}]$. This limit is then of the form $\ell(A \circ \pi_U)$ where ℓ is a uniquely defined probability measure on $[\dot{L}]$ which we call the *thermodynamic limit* of the ℓ_X:

$$\ell = \theta \lim\nolimits_{X\to\infty} \ell_X$$

This means that

$$\pi_U\ell = w^* \lim\nolimits_{X\to\infty} \pi_{UX}\ell_X$$

or (modulo the identifications $A \to A \circ \pi_{UX}$, $A \to A \circ \pi_U$) ℓ is the limit of the ℓ_X on

$$\cup_{U \text{ finite}} \mathcal{C}([\dot{U}] \mapsto \mathbf{R}) \circ \pi_U$$

which is dense in $\mathcal{C}([\dot{L}] \to \mathbf{R})$. In particular, if ℓ is any probability measure on $[\dot{L}]$, we have

$$\ell = \theta \lim\nolimits_{X\to\infty} \pi_X \ell$$

We shall later also consider thermodynamic limits associated with a sequence $X_n \to \infty$, writing $\ell = \theta \lim_{n\to\infty} \ell_{X_n}$ if $\pi_U\ell = w^* \lim_{n\to\infty} \pi_{UX_n}\ell_{X_n}$ for all finite $U \subset L$.

3.2 Proposition (time evolution of thermodynamic limits).

Suppose that

$$\theta\lim_{X\to\infty}\ell_X=\ell$$

where ℓ_X,ℓ are probability measures carried by $[X],[L]$ respectively. Then

$$\theta\lim_{X\to\infty}f_X^t\ell_X=f^t\ell$$

uniformly for $t\in[-T,T]$.

We have to prove that, for every finite $U\subset L$, and $A\in\mathcal{C}([\dot U]\to\mathbf{R})$,

$$\lim_{X\to\infty}(f_X^t\ell_X)(A\circ\pi_{UX})=(f^t\ell)(A\circ\pi_U)$$

We may (and shall) assume that $|A|\le 1$. Given $\epsilon>0$, we know that

$$||A\circ\pi_U\circ f^t-A\circ\pi_{UX}\circ f_X^t\circ\pi_X||<\frac{\epsilon}{2}$$

for sufficiently large X, say $X\supset V$ for suitable $V\supset U$, for all $t\in[-T,T]$. Under these conditions we have thus

$$||A\circ\pi_U\circ f^t-A\circ\pi_{UV}\circ f_V^t\circ\pi_V||<\epsilon/2$$

and

$$||A\circ\pi_{UX}\circ f_X^t\circ\pi_X-A\circ\pi_{UV}\circ f_V^t\circ\pi_V||<\epsilon$$

which we shall use below in the form

$$||A\circ\pi_{UX}\circ f_X^t-A\circ\pi_{UV}\circ f_V^t\circ\pi_{VX}||<\epsilon$$

Take now a function $\Phi\in\mathcal{C}([V]\to\mathbf{R})$ with compact support and $|\Phi|\le 1$, such that

$$||\ell-(\Phi\circ\pi_V)\ell||<\epsilon$$

Using the notation $a\overset{\epsilon}{\sim}b$ to mean $|a-b|<\epsilon$, we have

$$(f^t\ell)(A\circ\pi_U)\overset{\epsilon}{\sim}(f^t((\Phi\circ\pi_V)\ell))(A\circ\pi_U)=\ell((\Phi\circ\pi_V)(A\circ\pi_U\circ f^t))$$

$$\overset{\epsilon}{\sim}\ell((\Phi\circ\pi_V)(A\circ\pi_{UV}\circ f_V^t\circ\pi_V))=\ell((\Phi(A\circ\pi_{UV}\circ f_V^t))\circ\pi_V)=\ell(\Psi_t\circ\pi_V)$$

where the function $\Psi_t=\Phi(A\circ\pi_{UV}\circ f_V^t):[V]\to\mathbf{R}$ is continuous with compact support, hence extends to a continuous function on $[\dot V]$. By assumption we have

$$|\ell(\Psi_t\circ\pi_V)-\ell_X(\Psi_t\circ\pi_{VX})|<\epsilon$$

for sufficiently large X, uniformly with respect to $t \in [-T, T]$ (this is because $t \to \Psi_t$ is continuous with respect to the uniform norm of $\mathcal{C}([\dot{V}] \to \mathbf{R})$). We may thus take $W \supset V$ such that, if $X \supset W$ and $t \in [-T, T]$,

$$\ell(\Psi_t \circ \pi_V) \overset{\epsilon}{\sim} \ell_X(\Psi_t \circ \pi_{VX}) = \ell_X((\Phi(A \circ \pi_{UV} \circ f_V^t)) \circ \pi_{VX})$$

$$\overset{\epsilon}{\sim} \ell_X((\Phi \circ \pi_{VX})(A \circ \pi_{UX} \circ f_X^t)) = (f_X^t((\Phi \circ \pi_{VX})\ell_X))(A \circ \pi_{UX})$$

We have thus

$$|(f^t\ell)(A \circ \pi_U) - (f_X^t((\Phi \circ \pi_{VX})\ell_X))(A \circ \pi_{UX})| < 4\epsilon$$

when $X \supset W$, $t \in [-T, T]$. We may now let $\Phi \to 1$, obtaining

$$|(f^t\ell)(A \circ \pi_U) - (f_X^t \ell_X)(A \circ \pi_{UX})| \leq 4\epsilon$$

as announced. □

Proposition 3.2 also holds for the thermodynamic limit associated with a sequence $X_n \to \infty$

4 Γ-states and their time evolution.

We introduce now a special set of probability measures.

4.1 Definition (Γ-states).

We say that the probability measure ℓ carried by $[L]$ is a Γ-state if there exist constants $\tilde{\beta}_x > 0$ (for $x \in L$), smooth functions $\tilde{V}_x : \mathbf{T} \to \mathbf{R}$ (for $x \in L$) and $\tilde{W}_{\{x,y\}} : \mathbf{T} \times \mathbf{T} \to \mathbf{R}$ (for $\{x, y\} \in \Gamma$) such that the $\tilde{\beta}_x$, $\tilde{\beta}_x^{-1}$, $\tilde{V}_x$, $\tilde{W}_{\{x,y\}}$, $\partial_{q_x}\tilde{W}_{\{x,y\}}$, $\partial_{q_y}\tilde{W}_{\{x,y\}}$ are bounded uniformly in $x, y \in L$, and the following holds:

For every finite $X \subset L$, the conditional measure $\ell_X(d\xi|\eta)$ of ℓ on $[X]$ given $\eta \in [L\backslash X]$ is of the form

$$\ell_X(d\xi|\eta) = \text{const.} \exp[-\sum_{x\in X}(\frac{1}{2}\tilde{\beta}_x p_x^2 + \tilde{V}_x(q_x)) - \sum_{\{x,y\}}{}^{*}\,\tilde{W}_{\{x,y\}}(q_x, q_y)]\, d\xi$$

where $\sum^*$ extends over those $\{x, y\} \in \Gamma$ such that $x \in X$, and we have written $\xi = (p_x, q_x)_{x\in X}$, $\eta = (p_x, q_x)_{x\in L\backslash X}$.

[The Γ-states are *Gibbs states** for a certain interaction given by the $\tilde{\beta}_x$, $\tilde{V}_x$, $\tilde{W}_{\{x,y\}}$].

If ℓ is a Γ-state we may, for finite $U \subset L$, write $(\pi_U\ell)(d\xi) = \ell_U(\xi)d\xi$ where ℓ_U is smooth on $[U]$. Note that $\ell_U(\xi)$ has a (p, q)-factorization: it is the product of a smooth function of the q_x for $x \in U$, and of a Gaussian $\sqrt{\tilde{\beta}_x/2\pi}\exp(-\tilde{\beta}_x p_x^2/2)$ for each $x \in U$.

* See [14] for a discussion of Gibbs states in the simpler case of spin systems. We shall not make use of the theory of Gibbs states in the present paper.

We shall now take X finite and $Y = X \cup \tilde{X}_1 \cup \ldots \cup \tilde{X}_{\bar{k}}$, where

$$\tilde{X}_k = \{y \in L \backslash X : d(y, X) = k\}$$

($\bar{k}$ is thus the "size" of Y). If $\xi \in [X]$, and $\eta_k \in [\tilde{X}_k]$ for $k = 1, \ldots, \bar{k}$, the Γ-state property of ℓ then gives

$$\ell_Y(\xi, \eta_1, \ldots, \eta_{\bar{k}}) = C_{\bar{k}}.\ell_0(\xi|\eta_1).\ell_1(\eta_1|\eta_2) \cdots \ell_{\bar{k}-1}(\eta_{\bar{k}-1}, \eta_{\bar{k}}).\ell_{\bar{k}}(\eta_{\bar{k}})$$

where $C_{\bar{k}}$ is a normalization constant and (putting $\tilde{W}_{\{x,y\}} = 0$ if $\{x, y\} \notin \Gamma$):

$$\ell_0(\xi|\eta_1) = \exp[-\sum_{x \in X}(\tilde{\beta}_x p_x^2/2 + \tilde{V}_x(q_x)) - \sum_{x,y \in X} \tilde{W}_{\{x,y\}}(q_x, q_y) - \sum_{x \in X} \sum_{y \in \tilde{X}_1} \tilde{W}_{\{x,y\}}(q_x, q_y)]$$

$$\ell_k(\eta_k|\eta_{k+1}) = \exp[-\sum_{x \in \tilde{X}_k}(\tilde{\beta}_x p_x^2/2 + \tilde{V}_x(q_x)) - \sum_{x,y \in \tilde{X}_k} \tilde{W}_{\{x,y\}}(q_x, q_y)$$
$$- \sum_{x \in \tilde{X}_k} \sum_{y \in \tilde{X}_{k+1}} \tilde{W}_{\{x,y\}}(q_x, q_y)] \qquad \text{when } k > 0, \text{ and}$$

$$\ell_{\bar{k}}(\eta_{\bar{k}}) = \int \nu(d\eta_{\bar{k}+1})\, \ell_{\bar{k}}(\eta_{\bar{k}}|\eta_{\bar{k}+1}) \qquad \text{for some probability measure } \nu \text{ on } [\tilde{X}_{\bar{k}+1}].$$

Using the fact that the Jacobian of f_U^t is 1 (f_U^t preserves $d\xi$) we have

$$f_U^t((\pi_U \ell)(d\xi)) = f_U^t(\ell_U(\xi)d\xi) = \ell_U(f_U^{-t}\xi)d\xi$$

Thus, by Proposition 3.2, if $X \subset Y$ as above,

$$(\pi_X f^t \ell)(d\xi) = w^* \lim_{Y \to \infty} \pi_X(\ell_Y(f_Y^{-t}(\xi, \eta_Y))d\xi d\eta_Y)$$

We may write

$$f_Y^{-t}(\xi, \eta_Y) = (f_{Y0}^{-t}(\xi, \eta_Y), f_{Y1}^{-t}(\xi, \eta_Y), \ldots, f_{Y\bar{k}}^{-t}(\xi, \eta_Y))$$

with

$$f_{Y0}^{-t}(\xi, \eta_Y) \in [X], \qquad f_{Yk}^{-t}(\xi, \eta_Y) \in [\tilde{X}_k] \quad \text{for } k = 1, \ldots, \bar{k}$$

If $\xi, \tilde{\xi} \in [X]$, $\eta_Y \in [Y \backslash X]$, the quotient

$$\frac{\ell_Y(f_Y^{-t}(\xi, \eta_Y))}{\ell_Y(f_Y^{-t}(\tilde{\xi}, \eta_Y))}$$

is thus a product of quotients

$$\frac{\ell_k(f_{Yk}^{-t}(\xi, \eta_Y)|f_{Y(k+1)}^{-t}(\xi, \eta_Y))}{\ell_k(f_{Yk}^{-t}(\tilde{\xi}, \eta_Y)|f_{Y(k+1)}^{-t}(\tilde{\xi}, \eta_Y))} \qquad \text{for } k = 0, \ldots, \bar{k} - 1$$

and

$$\frac{\ell_{\bar{k}}(f^{-t}_{Y\bar{k}}(\xi,\eta_Y))}{\ell_{\bar{k}}(f^{-t}_{Y\bar{k}}(\tilde{\xi},\eta_Y))}$$

where the arguments $f^{-t}_{Yk}(\xi,\eta_Y)$, $f^{-t}_{Y(k+1)}(\xi,\eta_Y)$ and their derivatives have dependence on ξ that decreases faster than exponentially with respect to k (Propositions 2.7 and 2.8).

Let us define $\ell^t_{Yk}(\xi,\eta_Y)$ by

$$\ell_k(f^{-t}_{Yk}(\xi,\eta_Y)|f^{-t}_{Y(k+1)}(\xi,\eta_Y)) = \ell^t_{Yk}(\xi,\eta_Y).\exp\sum_{x\in\tilde{X}_k}(-\tilde{\beta}_x p_x(0)^2/2)$$

for $k=0,\ldots,\bar{k}-1$, where $\tilde{X}_k$ is replaced by X for $k=0$, and

$$\ell_{\bar{k}}(f^{-t}_{Y\bar{k}}(\xi,\eta_Y)) = \ell^t_{Y\bar{k}}(\xi,\eta_Y).\exp\sum_{x\in\tilde{X}_{\bar{k}}}(-\tilde{\beta}_x p_x(0)^2/2)$$

We shall also use $\ell^t_k(\xi,\eta)$ defined by

$$\ell_k(f^{-t}_k(\xi,\eta)|f^{-t}_{k+1}(\xi,\eta)) = \ell^t_k(\xi,\eta).\exp\sum_{x\in\tilde{X}_k}(-\tilde{\beta}_x p_x(0)^2/2)$$

where

$$f^{-t}(\xi,\eta) = (f^{-t}_0(\xi,\eta),\ldots,f^{-t}_k(\xi,\eta),\ldots)$$

with $f^{-t}_0(\xi,\eta)\in[X]$, and $f^{-t}_k(\xi,\eta)\in[\tilde{X}_k]$ for $k\geq 1$.

From our definitions it follows that

$$\frac{\ell_Y(f^{-t}_Y(\xi,\eta_Y))}{\ell_Y(f^{-t}_Y(\tilde{\xi},\eta_Y))} = \Big[\prod_{k=0}^{\bar{k}}\frac{\ell^t_{Yk}(\xi,\eta_Y)}{\ell^t_{Yk}(\tilde{\xi},\eta_Y)}\Big]\cdot\frac{\exp\sum_{x\in X}(-\tilde{\beta}_x p_x(0)^2/2)}{\exp\sum_{x\in X}(-\tilde{\beta}_x \tilde{p}_x(0)^2/2)}$$

4.2 Lemma (basic uniform estimates).

In the above formula, we have, uniformly in $t\in[-T,T]$ and the size $\bar{k}$ of Y, the estimates

(*a*)
$$|\log\ell^t_{Y0}(\xi,\eta_Y)| < \text{const.}(1+\sup_{x\in X}|p_x(0)|)$$

(*b*)
$$\Big|\log\frac{\ell^t_{Yk}(\xi,\eta_Y)}{\ell^t_{Yk}(\tilde{\xi},\eta_Y)}\Big| < \frac{\text{polyn.}(k)}{k!}(1+\sup_{x\in\tilde{X}_k}|p_x(0)|) \qquad \text{if } k\geq 1$$

These estimates remain true when ℓ^t_{Yk} is replaced by ℓ^t_k.

We note that, by Lemma 2.1(a),

$$|p_x(t)^2 - p_x(0)^2| \le K|t|(2|p_x(0)| + K|t|)$$

From this, and the definitions, the first inequality of the lemma follows. The second inequality is obtained by using also the finite dimensionality Assumption 1.1 and Lemma 2.1(b). ∎

Define now the regions $R_u, R_v^\times \subset [L] = [X] \times [L\backslash X]$ such that

$$R_u = \{(\xi,\eta) : |p_x| \le u \text{ if } x \in X\} \qquad , \qquad R_v^\times = \{(\xi,\eta) : |p_x| \le kv \text{ if } x \in \tilde{X}_k \text{ for } k \ge 1\}$$

4.3 Lemma (existence of limit in $R_u \cap R_v^\times$).

In $R_u \cap R_v^\times$, the expression

$$\frac{\ell_Y(f_Y^{-t}(\xi,\eta_Y))}{\int_{[X]} d\tilde\xi\,\ell_Y(f_Y^{-t}(\tilde\xi,\eta_Y))} \cdot [\ell_{Y0}^t(\xi,\eta_Y)\exp\sum_{x\in X}(-\tilde\beta_x p_x(0)^2/2)]^{-1}$$

$$= \Big[\int_{[X]} d\tilde\xi\,[\prod_{k=1}^{\bar k}\frac{\ell_{Yk}^t(\tilde\xi,\eta_Y)}{\ell_{Yk}^t(\xi,\eta_Y)}]\,\ell_{Y0}^t(\tilde\xi,\eta_Y)\exp\sum_{x\in X}(-\tilde\beta_x\tilde p_x(0)^2/2)\Big]^{-1}$$

has upper and lower bounds $\exp(\pm\text{const.}(1+v))$ *uniformly in u, $t \in [-T,T]$, and $\bar k$, and tends when $\bar k \to \infty$, uniformly for $(\xi,\eta) \in R_u \cap R_v^\times$, to*

$$\Big[\int_{[X]} d\tilde\xi\,[\prod_{k=1}^{\infty}\frac{\ell_k^t(\tilde\xi,\eta)}{\ell_k^t(\xi,\eta)}]\,\ell_0^t(\tilde\xi,\eta)\exp\sum_{x\in X}(-\tilde\beta_x\tilde p_x(0)^2/2)\Big]^{-1}$$

The limit is continuous.

Let $(\xi,\eta) \in R_u \cap R_v^\times$, and assume $\bar k$ to be large. The quotients

$$\frac{\ell_{Yk}^t(\tilde\xi,\eta_Y)}{\ell_{Yk}^t(\xi,\eta_Y)} \qquad (k \ge 1)$$

are nearly independent of Y (*i.e.*, of $\bar k$) for small k, and (using Lemma 4.2) very close to 1 for large k, so that

$$\lim_{\bar k\to\infty}\prod_{k=1}^{\bar k}\frac{\ell_{Yk}^t(\tilde\xi,\eta_Y)}{\ell_{Yk}^t(\xi,\eta_Y)} = \prod_{k=1}^{\infty}\frac{\ell_k^t(\tilde\xi,\eta)}{\ell_k^t(\xi,\eta)}$$

uniformly, and we have bounds $\exp(\pm\text{const.}(1+v))$ by Lemma 4.2(b). Note now that $\ell_{Y0}^t(\tilde\xi,\eta_Y)$ tends to $\ell_0^t(\tilde\xi,\eta)$ uniformly for $(\tilde\xi,\eta) \in R_u \cap R_v^\times$, and we can extend the integral over $\tilde\xi$ from $|p_x| < u$ to $[X]$ because the Gaussian

$$\exp\sum_{x\in X}(-\tilde\beta_x\tilde p_x(0)^2/2)$$

beats the exponential growth of $\ell^t_{Y0}(\tilde{\xi}, \eta_Y)$ given by Lemma 4.2(a). Bounds of the form $\exp(\pm\text{const.}(1+v))$ hold again after integration. ∎

4.4 Lemma (large v Gaussian estimate).

For large v, $(\pi_{Y\backslash X} f^t_Y \pi_Y \ell)(d\eta_Y)$ has mass $< \exp(-const.v^2)$ outside of $\pi_{Y\backslash X} R^\times_v$, uniformly in the size $\bar{k}$ of Y.

The (p,q)-factorization of $\ell_Y(\xi, \eta_Y)$ shows that the mass outside of $R^\times_v$ is bounded, uniformly in $\bar{k}$, by a Gaussian $< \exp(-\text{const}.v^2)$ for large v. But the time evolution f^t_Y changes $|p_x|$ (additively) by at most $K|t|$, so that the Gaussian estimate remains valid. ∎

4.5 Theorem (Smooth density of evolved states).

Let ℓ be a Γ-state. For finite X, and Y of size $\bar{k}$ as above, we write

$$\bar{\ell}^t_{YX}(\xi) \exp \sum_{x \in X} (-\tilde{\beta}_x p_x(0)^2/2) = \int d\eta_Y \, \ell_Y(f^{-t}_Y(\xi, \eta_Y))$$

There is a smooth function $\bar{\ell}^t_X(\xi)$ of ξ and t such that

$$(\pi_X f^t \ell)(d\xi) = \bar{\ell}^t_X(\xi) \exp \sum_{x \in X} (-\tilde{\beta}_x p_x(0)^2/2) \, d\xi$$

and we have, uniformly for $|p_x| < u$ $(x \in X)$ and $|t| \leq T$,

$$\bar{\ell}^t_X(\xi) = \lim_{\bar{k} \to \infty} \bar{\ell}^t_{YX}(\xi)$$

The limit also holds for the derivatives with respect to ξ, t. The $\bar{\ell}^t_X(\xi)$, $\bar{\ell}^t_{YX}(\xi)$ have upper and lower bounds $\exp(\pm\text{const.}(1+u))$, and the absolute values of their derivatives have bounds $\text{polyn.}(u).\exp(\text{const.}(1+u))$ uniformly in $t \in [-T, T]$ and $\bar{k}$.

We start with the remark that

$$\frac{\ell_Y(f^{-t}_Y(\xi, \eta_Y)) \, d\xi}{\int_{[X]} d\tilde{\xi} \, \ell_Y(f^{-t}_Y(\tilde{\xi}, \eta_Y))}$$

is the conditional measure of $f^t_Y \pi_Y \ell$ on $[X]$ given $\eta_Y \in [Y \backslash X]$. Integrating this conditional measure with respect to $(\pi_{Y\backslash X} f^t_Y \pi_Y \ell)(d\eta_Y)$ yields $\pi_X f^t_Y \pi_Y \ell$. Thus

$$\bar{\ell}^t_{YX}(\xi) = \int (\pi_{Y\backslash X} f^t_Y \pi_Y \ell)(d\eta_Y) \frac{\ell_Y(f^{-t}_Y(\xi, \eta_Y))}{\int_{[X]} d\tilde{\xi} \, \ell_Y(f^{-t}_Y(\tilde{\xi}, \eta_Y))} \cdot \exp \sum_{x \in X} (\tilde{\beta}_x p_x(0)^2/2)$$

The integrand in the right-hand side is the product of a factor controlled by Lemma 4.3, and a factor $\ell^t_{Y0}(\xi, \eta_Y)$ which has upper and lower bounds $\exp(\pm\text{const.}(1+u))$ uniformly in $\bar{k}$ (by Lemma 4.2(a)) and tends to $\ell^t_0(\xi, \eta)$ when $\bar{k} \to \infty$, uniformly for $(\xi, \eta) \in R_u \cap R^\times_v$.

Using also Lemma 4.4 and the fact that $\pi_{Y\backslash X} f_Y^t \pi_Y \ell$ has the w^*limit $\pi_{L\backslash X} f^t \ell$ when $\bar{k} \to \infty$ (Proposition 3.2) we find that

$$\lim_{\bar{k}\to\infty} \bar{\ell}^t_{YX}(\xi)$$

$$= \int (\pi_{L\backslash X} f^t \ell)(d\eta)\, \ell_0^t(\xi,\eta) \Big[\int_{[X]} d\tilde{\xi}\, [\prod_{k=1}^{\infty} \frac{\ell_k^t(\tilde{\xi},\eta)}{\ell_k^t(\xi,\eta)}]\, \ell_0^t(\tilde{\xi},\eta) \exp \sum_{x\in X} (-\tilde{\beta}_x \tilde{p}_x(0)^2/2) \Big]^{-1}$$

uniformly when $|p_x(0)| \leq u$ for $x \in X$, with uniform upper and lower bounds exp($\pm$const. $(1+u)$). We call the limit $\bar{\ell}^t_X(\xi)$. Since

$$\bar{\ell}^t_{YX}(\xi) \exp \sum_{x\in X} (-\tilde{\beta}_x p_x(0)^2/2)\, d\xi = (\pi_X f_Y^t \pi_Y \ell)(d\xi)$$

has the w^* limit $(\pi_X f^t \ell)(d\xi)$, it follows that this limit has a density

$$\bar{\ell}^t_X(\xi) \exp \sum_{x\in X} (-\tilde{\beta}_x p_x(0)^2/2)$$

as asserted.

Using the notation

$$f^t(\hat{\xi},\eta) = (f_0^t(\hat{\xi},,\eta), f^t_{\hat{\xi}}(\eta))$$

we may write

$$\bar{\ell}^t_X(\xi) = \int (f^t\ell)(d\hat{\xi}\, d\eta) \Big[\int_{[X]} d\tilde{\xi}\, [\prod_{k=1}^{\infty} \frac{\ell_k^t(\tilde{\xi},\eta)}{\ell_k^t(\xi,\eta)}]\, l_0^t(\tilde{\xi},\eta) \exp \sum_{x\in X} (-\tilde{\beta}_x \tilde{p}_x(0)^2/2) \Big]^{-1} l_0^t(\xi,\eta)$$

$$= \int \ell(d\hat{\xi}\, d\eta) \Big[\int_{[X]} d\tilde{\xi}\, [\prod_{k=1}^{\infty} \frac{\ell_k^t(\tilde{\xi}, f^t_{\hat{\xi}}(\eta))}{\ell_k^t(\xi, f^t_{\hat{\xi}}(\eta))}] l_0^t(\tilde{\xi}, f^t_{\hat{\xi}}(\eta)) \exp \sum_{x\in X} (-\tilde{\beta}_x \tilde{p}_x(0)^2/2) \Big]^{-1} l_0^t(\xi, f^t_{\hat{\xi}}(\eta))$$

and remember that this is the limit of a similar expression for $\bar{\ell}^t_{XY}(\xi)$. We want to show that $\bar{\ell}^t_X(\xi)$ has derivatives (of all orders) with respect to ξ, t by showing that the derivatives of $\bar{\ell}^t_{XY}(\xi)$, for ξ, t in a compact set, are bounded with respect to $\bar{k}$. Note that in estimating the integrals of polynomials in p, the $p_x(0)$ integral always has a Gaussian factor $\exp(-\beta_x p_x(0)^2/2)$ (remember the (p,q) factorization of ℓ). Therefore we only have to worry about bounding the coefficients of the polynomials.

Inspection of the above expression shows that computing a first order derivative essentially involves multiplying the integrand by the logarithmic derivatives of $l_0^t(\xi, f^t_{\hat{\xi}}(\eta))$, or $\ell_k^t(\tilde{\xi}, f^t_{\hat{\xi}}(\eta))/\ell_k^t(\xi, f^t_{\hat{\xi}}(\eta))$ and summing over k. In view of the very explicit form of the logarithm of the ℓ_k, we just have to estimate the derivatives of $f^{-t}(\xi, f^t_{\hat{\xi}}(\eta))$ with respect to ξ and t.

As far as $\ell_0^t(\xi, f^t_{\hat{\xi}}(\eta))$ is concerned, we have to consider the derivatives of $f_0^{-t}(\xi, f^t_{\hat{\xi}}(\eta))$ (or $f_1^{-t}(\xi, f^t_{\hat{\xi}}(\eta))$, which is similar). The ξ-derivative is of the form $r_x^{(0,1)}(-t; x_1)$ with

$x, x_1 \in X$, giving a bounded contribution by Proposition 2.7. The t-derivative is of the form

$$r_x^{(1,0)}(-t) + \sum_{x_1} r_x^{(0,1)}(-t; x_1) r_{x_1}^{(1,0)}(t)$$

with $x \in X$, and we may take $x_1 \in \tilde{X}_{k_1}$. By Proposition 2.7, $|r^{(0,1)}(\pm t)|$ is bounded by a polynomial in p with bounded coefficients, and $r_x^{(0,1)}(-t; x_1) \le \text{const.}/k_1!$, again giving a bounded contribution because $\sum_{k_1} |\tilde{X}_{k_1}|/k_1!$ is bounded.

We turn now to $\ell_k^t(\tilde{\xi}, f_{\hat{\xi}}^t(\eta))/\ell_k^t(\xi, f_{\hat{\xi}}^t(\eta))$, *i.e.*, we have to consider the derivatives of $f_k^{-t}(\xi, f_{\hat{\xi}}^t(\eta))$ (or f_{k+1}^{-t}). The ξ-derivative is of the form $r_x^{(0,1)}(-t; x_1)$ with $x \in \tilde{X}_k, x_1 \in X$, so that $|r_x^{(0,1)}(-t; x_1)| \le \text{const.}/d(x, x_1)! = \text{const.}/k!$, which makes a bounded contribution because $\sum_k |\tilde{X}_k|/k!$ is bounded. The t-derivative is of the form

$$\Delta r_x^{(1,0)}(-t; X) + \sum_{x_1} \Delta r_x^{(0,1)}(-t; x_1; X) r_{x_1}^{(1,0)}(t)$$

where $x \in \tilde{X}_k$ and we may take $x_1 \in \tilde{X}_{k_1}$. By Proposition 2.8 we have

$$|\Delta r_x^{(1,0)}(-t; X)| \le \text{polyn.}(p)/k!$$

$$|\Delta r_x^{(0,1)}(-t; x_1; X)| \le \text{const.}/\sigma! \le \text{const.}/\max(k, k_1)!$$

and since $\sum_k |\tilde{X}_k|/k!$, $\sum_{k,k_1} |\tilde{X}_k|.|\tilde{X}_{k_1}|/\max(k, k_1)!$ are bounded, we also have bounded contributions for the t-derivative.

We consider now higher order derivatives with respect to ξ, t. The computation of such a derivative gives terms where the integrand is multiplied by a product of logarithmic derivatives of the type discussed above; the contribution is again seen to be bounded. There are also terms containing derivatives of the logarithmic derivatives, and these are expressed in terms of higher order derivatives of $f^{-t}(\xi, f_{\hat{\xi}}^t(\eta))$ with respect to ξ, t. The derivative $\partial^j/\partial\xi_{x_1} \cdots \partial\xi_{x_j}$ is estimated by $|r_x^{(0,j)}(-t; x_1, \ldots, x_j)| \le \text{const.}/d(x, X)!$ giving a bounded contribution. The derivative $\partial^i/\partial t^i$ is a sum of terms $\Delta r_x^{(i_1,i_2)}(-t; y_1, \ldots, y_{i_2}; X)$ (multiplied by derivatives $\partial^k f_{\hat{\xi}}^t/\partial t^k = r^{(k,0)}$), where $i_1 + i_2 = i$; these terms can be estimated by Proposition 2.8, and give a bounded contribution. The general mixed derivative $\partial^{i+j}/\partial t^i \partial\xi_{x_1} \cdots \partial\xi_{x_j}$, with $j \ge 1$, is a sum of terms $r_x^{(i_1,j+i_2)}(-t; x_1, \ldots, x_j, y_1, \ldots, y_{i_2})$ with $x_1, \ldots, x_j \in X$ (multiplied by derivatives of the form $r^{(k,0)}$) which can be estimated by Proposition 2.7, and give a bounded contribution. $\square$

4.6 Remark (uniform bounds).

The proof of Theorem 4.5 gives estimates of $\bar{\ell}_{YX}^t(\xi)$ and its derivatives with respect to t and ξ, which are uniform with respect to the size $\bar{k}$ of Y. They are also uniform with respect to the Γ-states ℓ with conditional measures corresponding to a fixed choice of $\tilde{\beta}_x$, $\tilde{V}_x$, $\tilde{W}_{\{x,y\}}$, and remain uniform if some of the $\tilde{W}_{\{x,y\}}$ are replaced by 0.

For Y finite and $\eta = (p_x, q_x)_{x\in Y}$ define

$$\tilde\ell_Y(\eta) = Z_Y^{-1}\exp[-\sum_{x\in Y}(\frac{1}{2}\tilde\beta_x p_x^2 + \tilde V_x(q_x)) - \sum_{x,y\in Y}\tilde W_{\{x,y\}}(q_x, q_y)]$$

where Z_Y^{-1} is a normalization factor, and write

$$\bar{\tilde\ell}^t_{YX}(\xi)\exp\sum_{x\in X}(-\tilde\beta_x p_x(0)^2/2) = \int_{[Y\backslash X]} d\eta_Y\,\tilde\ell_Y(f_Y^{-t}(\xi,\eta_Y))$$

Then the above remarks show that the uniform estimates on $\bar\ell^t_{YX}(\xi)$ and its derivatives given by Theorem 4.5 can be taken to hold also for $\bar{\tilde\ell}^t_{YX}$.

5 Entropy.

Given a Γ-state ℓ, and $X\subset Y$ finite, we write

$$\pi_X f_Y^t \pi_Y \ell = \ell^t_{YX}(\xi)\,d\xi \qquad , \qquad \pi_X f^t\ell = \ell^t_X(\xi)\,d\xi$$

where $(t,\xi)\mapsto \ell^t_{YX}(\xi), \ell^t_X(\xi)$ are smooth on $\mathbf{R}\times[X]$.

In Theorem 4.5, we used the notation

$$\ell^t_{YX}(\xi) = \bar\ell^t_{YX}(\xi)\exp\sum_{x\in X}(-\tilde\beta_x p_x(0)^2/2) \qquad , \qquad \ell^t_X(\xi) = \bar\ell^t_X(\xi)\exp\sum_{x\in X}(-\tilde\beta_x p_x(0)^2/2)$$

and saw that $\bar\ell^t_{YX}(\xi)$ tends to $\bar\ell^t_X(\xi)$ together with its derivatives, uniformly on compacts of $\mathbf{R}\times[X]$, when $Y\to\infty$.

We can now define a (Gibbs) entropy $S^t_Y(X)$ or $S^t(X)$ by

$$S^t_Y(X) = -\int_{[X]}\ell^t_{YX}(\xi)\log\ell^t_{YX}(\xi)\,d\xi \qquad , \qquad S^t(X) = -\int_{[X]}\ell^t_X(\xi)\log\ell^t_X(\xi)\,d\xi$$

These are convergent integrals in view of the uniform bounds given in Theorem 4.5. Furthermore $S^t_Y(X)\to S^t(X)$, uniformly for $|t|\le T$, when $Y\to\infty$.

We may assume that $Y\supset\tilde X_1 = \{y\in L : \mathrm{dist}(y,X)=1\}$. If $\xi\in[X], \eta\in[Y\backslash X]$ or $[L\backslash X]$, let $\eta_1\in\tilde X_1$ be obtained from η by restricting the index set to $\tilde X_1$. Then the equations of motion for ξ,η show that we may write

$$\frac{d\xi}{dt} = \mathcal{X}(\xi,\eta_1) \qquad , \qquad \frac{d\eta}{dt} = \mathcal{Y}(\xi,\eta)$$

where $\mathcal{X}$ does not depend on Y. Writing $\hat\ell^t_Y = \ell_Y\circ f_Y^{-t}$, we have

$$\ell^t_{YX}(\xi) = \int_{[Y\backslash X]} d\eta\,\hat\ell^t_Y(\xi,\eta)$$

and the "continuity equation"

$$\frac{d}{dt}\hat{\ell}^t_Y(\xi,\eta) + \nabla_\xi \cdot (\hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)) + \nabla_\eta \cdot (\hat{\ell}^t_Y(\xi,\eta)\mathcal{Y}(\xi,\eta)) = 0$$

so that

$$\frac{d}{dt}\ell^t_{YX}(\xi) = -\int_{[Y\backslash X]} d\eta\, \nabla_\xi \cdot (\hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)) = -\nabla_\xi \cdot \int_{[Y\backslash X]} d\eta\, \hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)$$

$$\frac{d}{dt}\log \ell^t_{YX}(\xi) = -\frac{1}{\ell^t_{XY}(\xi)}\nabla_\xi \cdot \int_{[Y\backslash X]} d\eta\, \hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)$$

$$\frac{d}{dt}[\ell^t_{YX}(\xi)\log \ell^t_{YX}(\xi)] = -(\log \ell^t_{YX}(\xi)+1)\nabla_\xi \cdot \int_{[Y\backslash X]} d\eta\, \hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)$$

Using the estimates of Theorem 4.5 we find that $t \mapsto S^t_Y(X)$ is a smooth function of t, with

$$\begin{aligned}\frac{d}{dt}S^t_Y(X) &= \int_{[X]} d\xi\, \log \ell^t_{YX}(\xi)\, \nabla_\xi \cdot \int_{[Y\backslash X]} d\eta\, \hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1) \\ &= -\int_{[X]} \frac{d\xi}{\ell^t_{YX}(\xi)}(\nabla_\xi \ell^t_{YX}(\xi)) \cdot \int_{[Y\backslash X]} d\eta\, \hat{\ell}^t_Y(\xi,\eta)\mathcal{X}(\xi,\eta_1)\end{aligned}$$

Write now $X+ = X \cup \tilde{X}_1 = \{y \in L : d(y,X) \le 1\}$. The probability measure

$$\ell^t_{YX+}(\xi,\eta_1)\, d\xi\, d\eta_1$$

conditioned on $\xi \in [X]$ is denoted by $\ell^t_{YX+}(\eta_1|\xi)\, d\eta_1$ where

$$\ell^t_{YX+}(\eta_1|\xi) = \frac{\ell^t_{YX+}(\xi,\eta_1)}{\ell^t_{YX}(\xi)}$$

Theorem 4.5 gives uniform estimates for

$$\ell^t_{YX+}(\eta_1|\xi) \qquad , \qquad \nabla_\xi \ell^t_{YX+}(\eta_1|\xi)$$

so that

$$\begin{aligned}\frac{d}{dt}S^t_Y(X) &= -\int_{[X]} d\xi\, \nabla_\xi \ell^t_{YX}(\xi) \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{YX+}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1) \\ &= \int_{[X]} d\xi\, \ell^t_{YX}(\xi)\nabla_\xi \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{YX+}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1)\end{aligned}$$

It follows also that, when $Y \to \infty$, $dS^t_Y(X)/dt$ tends to

$$\int_{[X]} d\xi\, \ell^t_X(\xi)\nabla_\xi \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{X+}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1)$$

uniformly for $|t| \leq T$, and the limit is $dS^t(X)/dt$.

5.1 Proposition (time derivative of $S(X)$, X finite).

When $Y \to \infty$, the derivative $dS^t_Y(X)/dt$ tends, uniformly for $|t| \leq T$, to

$$\frac{d}{dt}S^t(X) = \int_{[X]} d\xi\, \ell^t_X(\xi)\nabla_\xi \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{X+}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1)$$

which is a smooth function of t.

The proof, as given above, is essentially a corollary of Theorem 4.5. $\square$

Suppose now that $\tilde{X}_1 = \{y \in L : d(x,y) = 1\}$ is finite, but X is not necessarily finite. We still have, for Y finite,

$$\frac{d}{dt}S^t_Y(X\cap Y) = \int_{[X\cap Y]} d\xi\, \ell^t_{Y,X\cap Y}(\xi)\nabla_\xi \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{Y,X+\cap Y}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1)$$

and this can be bounded independently of Y.

5.2 Proposition (time derivative of $\Delta S^t(X)$).

If $X \subset L$, and X is not necessarily finite, but $\tilde{X}_1 = \{y \in L : d(X,y) = 1\}$ is finite, we may define

$$\Delta S^t(X) = \lim_{Y\to\infty}(S^t(X\cap Y) - S^0(X\cap Y))$$

and we have

$$\frac{d}{dt}\Delta S^t_Y(X) = \int_{[X]} (\pi_X f^t\ell)(d\xi)\nabla_\xi \cdot \int_{[\tilde{X}_1]} d\eta_1\, \ell^t_{X+}(\eta_1|\xi)\mathcal{X}(\xi,\eta_1)$$

which is a smooth function of t.

This follows from the usual estimates. Note that ∇_ξ is a derivative with respect to a finite number of variables corresponding to nonzero components of $\mathcal{X}(\xi,\eta_1)$. $\square$

We shall now study a *conditional*, or "external" entropy $\check{S}$ defined for X finite by

$$\check{S}^t_Y(X) = S^t_Y(Y) - S^t_Y(Y\backslash X)$$

Using the notation

$$\hat{\ell}^t_Y = \ell_Y \circ f^{-t}_Y \qquad , \qquad \ell_{Y,Y\backslash X}(\eta) = \int_{[X]} d\xi\, \hat{\ell}^t_Y(\xi,\eta) \qquad , \qquad \ell^t_{YX}(\xi|\eta) = \frac{\hat{\ell}^t_Y(\xi,\eta)}{\ell_{Y,Y\backslash X}(\eta)}$$

as above, we find

$$\check{S}^t_Y(X) = -\int d\xi\, d\eta\, \hat{\ell}^t_Y(\xi,\eta) \log \frac{\hat{\ell}^t_Y(\xi,\eta)}{\ell_{Y,Y\backslash X}(\eta)}$$

$$= \int \ell_{Y,Y\backslash X}(\eta)\,d\eta[-\int d\xi\,\ell^t_{YX}(\xi|\eta)\log\ell^t_{YX}(\xi|\eta)] = \int \ell_{Y,Y\backslash X}(\eta)\,d\eta\,S^t_Y(X|\eta)$$

where we have written

$$S^t_Y(X|\eta) = -\int d\xi\,\ell^t_{YX}(\xi|\eta)\log\ell^t_{YX}(\xi|\eta)$$

Let also

$$\ell^t_X(\xi|\eta) = [\int_{[X]} d\tilde\xi[\prod_{k=1}^\infty \frac{\ell^t_k(\tilde\xi,\eta)}{\ell^t_k(\xi,\eta)}]\ell^t_0(\tilde\xi,\eta)\exp\sum_{x\in X}(-\tilde\beta_x\tilde p_x(0)^2/2)]^{-1}$$

$$\times\ell^t_0(\xi,\eta)\exp\sum_{x\in X}(-\beta_x p_x(0)^2/2)$$

$$S^t(X|\eta) = -\int d\xi\,\ell^t_X(\xi|\eta)\log\ell^t_X(\xi|\eta)$$

then Lemma 4.2(a) and Lemma 4.3 imply that $S^t_Y(X|\eta)\to S^t(X|\eta)$ when $Y\to\infty$, uniformly for $\eta\in\pi_{L\backslash X}R^\times_v$ and $t\in[-T,T]$, and with uniform bounds

$$|S^t_Y(X|\eta)| \le \text{const.}(1+v)$$

Therefore (using Lemma 4.4 and Proposition 3.2)we see that when $Y\to\infty$ we have

$$\check S^t_Y(X) \to \check S^t(X)$$

uniformly for $t\in[-T,T]$, where

$$\check S^t(X) = \int(\pi_{L\backslash X}f^t\ell)(d\eta)\,S^t(X|\eta)$$

Note that $\check S^t(X)$ is obtained by taking the mean entropy $S^t(X|\eta)$ associated with $\ell^t_X(\xi|\eta)$ and averaging over η, while $S^t(X)$ is the entropy associated with the average $\ell_X(\xi)$ of $\ell^t_X(\xi|\eta)$ over η. In particular, concavity gives $\check S^t(X)\le S^t(X)$.

Since $dS^t_Y(Y)/dt = 0$, we have

$$\frac{d}{dt}\check S^t_Y(X) = -\frac{d}{dt}S^t_Y(Y\backslash X)$$

$$= -\int_{[Y\backslash X]} d\eta\,\ell^t_{Y,Y\backslash X}(\eta)\nabla_\eta\cdot\int_{[X]} d\xi\,\ell^t_{YX}(\xi|\eta)\mathcal{Y}(\xi,\eta)$$

$$= -\int_{[Y\backslash X]} d\eta\,\ell^t_{Y,Y\backslash X}(\eta)\sum_{y\in\tilde X_1}\partial_{\eta_y}\cdot\int_{[X]} d\xi\,\ell^t_{YX}(\xi|\eta)\mathcal{Y}_y(\xi,\eta)$$

where $\tilde X_1 = \{y\in Y : d(y,X)=1\}$ and $\mathcal{Y}_y$ is the y-component of $\mathcal{Y}$. We may now let $Y\to\infty$, finding:

5.3 Proposition (time derivative of the entropy $\check{S}$).

When $Y \to \infty$, the derivative $d\check{S}^t_Y(X)/dt$ tends, uniformly for $t \in [-T, T]$, to

$$\frac{d}{dt}\check{S}^t(X) = -\int (\pi_{L\backslash X} f^t \ell)(d\eta) \sum_{y \in \tilde{X}_1} \partial_{\eta_y} \cdot \int_{[X]} d\xi\, \ell^t_X(\xi|\eta) \mathcal{Y}_y(\xi, \eta)$$

which is a smooth function of t.

This is again a corollary of Theorem 4.5. □

Note that

$$\frac{d}{dt}\check{S}^t(X) = -\frac{d}{dt}\Delta S^t(L\backslash X)$$

5.4 Assumption (bounded energy).

For every finite $X \subset L$ the kinetic energy is bounded independently of t:

$$\int d\xi\, \ell^t_X(\xi) p_X^2/2 \le \text{const.}(X)$$

[it would be equivalent to assume a bound on the total energy H_X].

We have the general inequality

$$S^t(X) \le \int d\xi\, \ell^t_X(\xi) p_X^2/2 + |X| \log \sqrt{2\pi}$$

[this follows from the "variational principle for the free energy", and can be proved by using the concavity of the log:

$$\int d\xi\, \ell^t_X(\xi) \log \frac{e^{-p_X^2/2}}{\ell^t_X(\xi)} \le \log \int d\xi\, e^{-p_X^2/2} = |X| \log \sqrt{2\pi} \qquad]$$

Therefore the bounded energy assumption gives a bound on the entropy:

$$S^t(X) \le \text{const.}(X)$$

Similarly, we find

$$S^t(X|\eta) \le \int d\xi\, \ell^t_X(\xi|\eta) p_X^2/2 + |X| \log \sqrt{2\pi}$$

hence

$$\check{S}^t(X) \le \int d\xi\, \ell^t_X(\xi) p_X^2/2 + |X| \log \sqrt{2\pi} \le \text{const.}(X)$$

In particular we have $\check{S}^t(X) \le S^t(X) \le \text{const.}(X)$.

5.5 Definitions (large volume limit).

We may take a sequence (T_n) tending to $+\infty$ such that $\frac{1}{T_n}\int_0^{T_n} dt\, f^t\ell$ has a limit ρ in the vague topology of measures on $[\dot{L}]$:

$$t_n \to \infty \qquad , \qquad \frac{1}{T_n}\int_0^{T_n} dt\, f^t\ell \to \rho$$

We call the probability measure ρ a *nonequilibrium steady state* (NESS). In view of Assumption 5.4, ρ is carried by $[L]$. Furthermore ρ is invariant under (f^t).

We can also (by going to a subsequence) assume that

$$\frac{\Delta S^{T_n}(X)}{T_n} = \frac{1}{T_n}\int_0^{T_n} dt\, \frac{d}{dt}\Delta S^t(X) \to \sigma(X)$$

when $\tilde{X}_1 = \{y \in L : d(X,y) = 1\}$ is finite (X need not be finite). Note that $\sigma(X)$ might not be determined by ρ and X.

For notational simplicity we shall write $T \to \infty$ instead of $T_n, n \to \infty$.

5.6 Interpretation (entropy production). [16]

As mentioned in the Introduction, Denis Evans and coworkers [16] have proposed to identify the mean entropy production rate in a finite region X to

$$e(X) = -\sigma(X) = -\lim_{T\to\infty} \frac{S^T(X) - S^0(X)}{T}$$

According to Proposition 5.1 this is the mean rate of volume contaction in $[X]$, and $e(X)$ corresponds to the accepted definition of entropy production in the presence of a deterministic thermostat.

A related choice is

$$\check{e}(X) = \sigma(L\backslash X) = -\lim_{T\to\infty} \frac{\check{S}^T(X) - \check{S}^0(X)}{T}$$

This is the mean rate of volume expansion in $[L\backslash X]$, and corresponds to the rate of entropy growth due to X, as seen by the "external world" $L\backslash X$.

Since $\check{S}^t(X) \le S^t(X) \le \text{const.}(X)$, we have $0 \le e(X) \le \check{e}(X)$.

We may also define mean entropy production rates associated with a finite partition $\mathcal{A} = (X_0, X_1, \ldots, x_n)$ of L provided $X_0, X_1, \ldots, X_n$ have finite "boundaries" $\{y \in L : d(X_i, y) = 1\}$. We write

$$e(\mathcal{A}) = \sum_{j=0}^{n} \sigma(X_j) \qquad , \qquad \check{e}(\mathcal{A}) = \sum_{j:X_j \text{ infinite}} \sigma(X_j)$$

In particular, in Case II, for X finite $\supset X_0$, we have

$$\check{e}(X) = \check{e}((X, L\backslash X)) \leq \check{e}((X, L_1\backslash X, L_2\backslash X))$$

We proceed now with some general inequalities satisfied by σ, e, and $\check{e}$.

5.7 Basic inequalities.

We have $e(\emptyset) = \check{e}(\emptyset) = 0$ by definition, and remember that $0 \leq e(X) \leq \check{e}(X)$. The strong subadditivity of the entropy implies that, if U, V have finite boundaries,

$$\sigma(U \cup V) - \sigma(U) - \sigma(V) + \sigma(U \cap V) \leq 0$$

(we have used the fact that $S^0((U \cup V) \cap Y) - S^0(U \cap Y) - S^0(V \cap Y) + S^0(U \cap V \cap Y)$ is bounded independently of Y). This implies the strong superadditivity of e, and subadditivity of $\check{e}$. In particular

$$e(U \cup V) \geq e(U) + e(V) \qquad \text{if} \qquad U \cap V = \emptyset$$

and

$$\check{e}(U \cup V) \leq \check{e}(U) + \check{e}(V)$$

If $U \subset V$ we also have*

$$e(U) \leq e(V) \qquad , \qquad \check{e}(U) \leq \check{e}(V)$$

i.e., $e(X), \check{e}(X)$ are increasing functions of X.

We can extend the definition of $e(X), \check{e}(X)$ to infinite X:

$$e(X) = \sup_{\text{finite}\, U \subset X} e(U) \qquad , \qquad \check{e}(X) = \sup_{\text{finite}\, U \subset X} \check{e}(U)$$

In the situations of interest for us $\check{e}(L)$ will be finite and we may call this quantity the *total entropy production rate*. Note that the entropy production rate $\check{e}(X)$ is not an additive function of X, but that its subadditivity amounts to some kind of locality. Note also that if $e(X) > 0$ we must have $S^T(X) \to -\infty$, in particular the ℓ_X^T cannot remain bounded when $T \to \infty$, contrary to some evidence [4], [5]. But there is no obvious objection to having an entropy production rate $\check{e}(X) > 0$.

6 Thermodynamic bound on entropy production.

We shall show that in Case I (an external force and a thermostat at temperature β^{-1}) we have

$$\check{e}(X) \leq \beta \times \text{energy flux to thermostat}$$

* Note that, for $U \subset V$, we have $S_Y^T(Y\backslash U) \leq S_Y^T(Y\backslash V) + S_Y^T(V\backslash U)$, hence $\check{S}_Y^T(V) \leq \check{S}_Y^T(U) + S_Y^T(V\backslash U)$, hence $\check{e}(V) \geq \check{e}(U) + e(V\backslash U)$.

where the right-hand side is the thermodynamic rate of entropy production. A more general result is given below (see Proposition 6.3).

In Case I we have introduced a finite set X_0 on which external forces act. As initial state ℓ we shall use the thermodynamic limit of a sequence:

$$\ell = \theta \lim_{Y\to\infty}\tilde{\ell}_Y(\eta)\, d\eta$$

where*

$$\tilde{\ell}_Y(\eta) = Z_Y^{-1} \exp[-\tilde{H}_{X_0} - \beta H_{Y\backslash X_0}]$$

In this formula,

$$\tilde{H}_{X_0} = \sum_{x\in X_0} (\frac{1}{2}\,\tilde{\beta}_x p_x^2 + \tilde{V}_x) + \sum_{x,y\in X_0} \tilde{W}_{\{x,y\}}$$

$$H_{Y\backslash X} = \sum_{x\in Y\backslash X} (\frac{1}{2}\,p_x^2 + V_x) + \sum_{x,y\in Y\backslash X} W_{\{x,y\}}$$

and Z_Y^{-1} is a normalization factor. In this section it will be convenient to use X_0 instead of X in the definition of Y, so that $Y = X_0 \cup \tilde{X}_1 \cup \ldots \cup \tilde{X}_{\bar{k}}$. We take X of the form $X_0 \cup \tilde{X}_1 \cup \ldots \cup \tilde{X}_k$ (this is no serious restriction) and choose a subsequence $\bar{k} \to \infty$ such that the $\pi_{XY}(\tilde{\ell}_Y(\eta)\, d\eta)$ converge vaguely (we use here the thermodynamic limit for a sequence as explained in Section 3).

The state ℓ is a Γ-state corresponding to the choice $\tilde{\beta}_x = \beta$, $\tilde{V}_x = \beta V_x$ for $x \notin X_0$, and $\tilde{W}_{\{x,y\}} = \beta W_{\{x,y\}}$ for $x, y \notin X_0$. We define

$$\tilde{\ell}^t_{YX}(\xi) = \int_{[Y\backslash X]} \tilde{\ell}_Y(f_Y^{-t}(\xi, \eta_Y))\, d\eta_Y$$

and

$$\tilde{S}^t_Y(X) = -\int_{[X]} \tilde{\ell}^t_{YX}(\xi) \log \tilde{\ell}^t_{YX}(\xi)\, d\xi \qquad , \qquad \check{\tilde{S}}^t_Y(X) = \tilde{S}^t_Y(Y) - \tilde{S}^t_Y(Y\backslash X)$$

Writing

$$\tilde{\ell}^t_{YX}(\xi|\eta) = \tilde{\ell}^t_{YY}(\xi, \eta)/\tilde{\ell}_{Y,Y\backslash X}(\eta)$$

$$\tilde{S}^t_Y(X|\eta) = -\int d\xi\, \tilde{\ell}^t_{YX}(\xi|\eta) \log \tilde{\ell}^t_{YX}(\xi|\eta)$$

we find

$$\check{\tilde{S}}^t_Y(X) = \int \tilde{\ell}^t_{Y,Y\backslash X}(\eta) d\eta\, \tilde{S}^t_Y(X|\eta)$$

* More generally we could allow a term $\sum_{x\in X_0, y\notin X_0} \tilde{W}_{\{x,y\}}$ of interaction between X_0 and $Y\backslash X_0$.

6.1 Lemma (thermodynamic limit for $\check{\tilde{S}}$).

$$\check{\tilde{S}}^t_Y(X) \to \check{S}^t(X)$$

together with the t-derivatives, uniformly for $t \in [-T, T]$, when $\bar{k} \to \infty$.

We have shown (in the proof of Proposition 5.2) how $\check{S}^t_Y(X) \to \check{S}^t(X)$. We proceed in the same way here, using the uniform estimates of Theorem 4.5 which hold again when ℓ is replaced by $\tilde{\ell}$, as explained in Remark 4.6. $\square$

Since f^t_Y is volume preserving in $[Y]$ we have

$$\tilde{S}^t_Y(Y) = \tilde{S}^0_Y(Y)$$

therefore

$$\check{\tilde{S}}^0_Y(X) - \check{\tilde{S}}^t_Y(X) = \tilde{S}^t_Y(Y\backslash X) - \tilde{S}^0_Y(Y\backslash X)$$

We fix now X, with $X_0 \subset X \subset Y$ as indicated above. Note that, by the (p, q) factorization, $\tilde{S}^0_Y(Y\backslash X_0) = \tilde{S}_{Y\backslash X_0}(Y\backslash X_0)$ is the sum of a momentum term $\tilde{S}^{0p}$ (integral over p, trivial) and a configuration term $\tilde{S}^{0q}$ (integral over q). The configuration part $\tilde{\ell}^q_{Y,Y\backslash X}(q_{Y\backslash X})$ of $\tilde{\ell}_{Y,Y\backslash X}(q_{Y\backslash X})$ differs from $\tilde{\ell}_{Y,Y\backslash X_0}(q_Y) = \tilde{\ell}^q_{Y\backslash X_0}(q_{X\backslash X_0}(q_{Y\backslash X})$ by a factor bounded independently of Y (because there is a finite number of bounded terms $\tilde{V}_x$ and $\tilde{W}_{\{x,y\}}$ with $x \in X\backslash X_0$). Therefore $|\log \tilde{\ell}^q_{Y,Y\backslash X}(q_{Y\backslash X}) - \log \tilde{\ell}^q_{Y\backslash X_0}(q_Y)|$ is bounded independently of Y, hence $|\tilde{S}^0_Y(Y\backslash X_0) - \tilde{S}^0_Y(Y\backslash X)| \leq C_0$ with C_0 independent of Y. Define now a function ℓ^* on $[Y\backslash X_0] = [X\backslash X_0] \times [Y\backslash X]$ to be the product of

$$Z^{-1} \exp(-\beta p^2_{X\backslash X_0}/2)$$

on $[X\backslash X_0]$ (with Z^{-1} a normalization factor) and $\tilde{\ell}^t_{Y,Y\backslash X}$ on $[Y\backslash X]$. Then there is a constant C_1 such that

$$S^* = -\int_{[Y\backslash X_0]} d\eta\, \ell^*(\eta) \log \ell^*(\eta) = \tilde{S}^t_Y(Y\backslash X) + C_1$$

and the "variational principle for the free energy" gives

$$S^* - \tilde{S}^0_Y(Y\backslash X_0) \leq \int_{[Y\backslash X_0]} d\eta\, (\ell^*(\eta) - \tilde{\ell}_{Y\backslash X_0}(\eta))\, \beta H_{Y\backslash X_0}(\eta)$$

so that

$$\tilde{S}^t_Y(Y\backslash X) - \tilde{S}^0_Y(Y\backslash X) \leq C_0 - C_1 + S^* - \tilde{S}^0_Y(Y\backslash X)$$

$$\leq C_0 - C_1 + \int_{[Y\backslash X_0]} d\eta\, (\ell^*(\eta) - \tilde{\ell}_{Y\backslash X_0}(\eta))\, \beta H_{Y\backslash X_0}(\eta)$$

There are also constants C_2, C_3 such that

$$\int_{[Y\setminus X_0]} d\eta\, \ell^*(\eta)\beta H_{Y\setminus X_0}(\eta) \leq \int_{[Y\setminus X]} d\eta\, \tilde{\ell}^t_{Y,Y\setminus X}(\eta)\beta H_{Y\setminus X}(\eta) + C_2$$

$$\int_{[Y\setminus X_0]} d\eta\, \tilde{\ell}_{Y\setminus X_0}(\eta))\, \beta H_{Y\setminus X_0}(\eta) \geq \int_{[Y\setminus X]} d\eta\, \tilde{\ell}^0_{Y,Y\setminus X}(\eta)\beta H_{Y\setminus X}(\eta) + C_3$$

Therefore, with a constant $C = C_0 - C_1 + C_2 - C_3$ independent of Y and t, we have

$$\check{\tilde{S}}^0_Y(X) - \check{\tilde{S}}^t_Y(X) \leq C + \int_{[Y\setminus X]} d\eta[\tilde{\ell}^t_{Y,Y\setminus X}(\eta) - \tilde{\ell}^0_{Y,Y\setminus X}(\eta)]\beta H_{Y\setminus X}(\eta)$$

$$= C + \beta \int_{[Y]} d\eta\, [\tilde{\ell}^t_Y(\eta) - \tilde{\ell}^0_Y(\eta)] H_{Y\setminus X}(\eta)$$

$$= C + \beta \int_{[Y]} d\eta\, \tilde{\ell}^0_Y(\eta)[H_{Y\setminus X}(f^t_Y\eta) - H_{Y\setminus X}(\eta)]$$

$$= C + \beta \int_{[Y]} d\eta\, \tilde{\ell}^0_Y(\eta) \int_0^t d\tau\, \frac{d}{d\tau} H_{Y\setminus X}(f^\tau_Y\eta)$$

The equations of motion yield

$$\frac{d}{d\tau} H_{Y\setminus X}(f^\tau_Y\eta) = \Phi(\pi_{X+,Y} f^\tau_Y\eta)$$

where $X+ = \{x \in L : d(x, X) \leq 1\}$ and $\Phi(p_Y, q_Y)$ is given by

$$\Phi = -\sum_{x\in X}\sum_{y\notin X} p_y \frac{\partial}{\partial q_y} W_{\{x,y\}}(q_x, q_y)$$

Therefore

$$\int_{[Y]} d\eta\, \tilde{\ell}^0_Y(\eta) \int_0^t d\tau\, \Phi(\pi_{X+,Y} f^\tau_Y\eta) = \int_0^t d\tau \int_{[Y]} d\eta\, \tilde{\ell}^\tau_Y(\eta)\Phi(\pi_{X+,Y}\eta)$$

$$= \int_0^t d\tau \int_{[X+]} d\xi\, \tilde{\ell}^\tau_{YX+}(\xi)\Phi(\xi)$$

so that

$$\check{\tilde{S}}^0_Y(X) - \check{\tilde{S}}^t_Y(X) \leq C + \beta \int_0^t d\tau \int_{[X+]} d\xi\, \tilde{\ell}^\tau_{YX+}(\xi)\Phi(\xi)$$

We may now let $Y \to \infty$, obtaining

$$\check{S}^0(X) - \check{S}^t(X) \leq C + \beta \int_0^t d\tau \int_{[X+]} d\xi\, \ell^\tau_{X+}(\xi)\Phi(\xi)$$

6.2 Proposition (bound on entropy production, Case I).

In case I the mean rate of entropy production of the finite set X is $\leq \beta \times$energy flux out of X_0:

$$0 \leq \check{e}(X) \leq \beta \int (\pi_{X_0+}\rho)(d\xi)\Phi_0(\xi)$$

where Φ_0 is the function Φ computed for $X = X_0$.

It suffices to consider the case of large X, so we assume $X \supset X_0$. Taking in the previous inequality the large time limit described in 5.4 we obtain

$$0 \leq \check{e}(X) \leq \beta \int (\pi_{X+}\rho)(d\xi)\,\Phi(x)$$

where the right-hand side is independent of X, and we may thus take $X = X_0$. $\square$

We now give without proof a general bound on $\sigma(X)$, which can be obtained using the same ideas as for Proposition 6.2.

6.3 Proposition. (bound on $\sigma(X)$).

Let X be infinite, with finite "boundary" $\tilde{X}_1 = \{y \in L : d(X,y) = 1\}$. we let the initial state ℓ be the thermodynamic limit of a sequence:

$$\ell = \theta \lim_{Y\to\infty} \tilde{\ell}_Y(\eta)\,d\eta$$

where

$$\tilde{\ell}_Y(\eta) = Z_Y^{-1} e^{-\tilde{H}_Y}$$

$$\tilde{H}_Y = \sum_{x\in Y}(\frac{1}{2}\tilde{\beta}_x p_x^2 + \tilde{V}_x) + \sum_{x,y\in Y}\tilde{W}_{\{x,y\}}$$

We assume that

$$\tilde{\beta}_x = \beta \qquad , \qquad \tilde{V}_x = \beta V_x \qquad , \qquad \tilde{W}_{\{x,y\}} = \beta W_{\{x,y\}}$$

when $x, y \in X$, i.e., X is a thermostat at temperature β^{-1}. Then

$$\sigma(X) \leq \beta \times \text{energy flux to } X$$

Note that if the energy flows out of X, then $\sigma(X) < 0$, and in particular $\sigma(X)$ does not vanish. Applications of Proposition 6.3, in particular to Case II, are left to the reader.

A Appendices.

A.1 (proof of Proposition 2.7).

By uniformity of the bounds it suffices to consider the situation when Y is finite. The case $(i,j)=(0,0)$ follows from Lemma 2.1(a), with $\tau=\sigma=0$.

Differentiating the time evolution equation for $\eta_x(t)=(p_x(t),q_x(t))$, we find

$$\frac{d}{dt}r_x^{(0,1)}=\sum_{y\in B_x^1}\Phi_{xy}(q_x,q_y)r_y^{(0,1)}$$

where Φ_{xy} depends smoothly on the q's, is independent of the p's, and there is a uniform bound

$$\sum_y|\Phi_{xy}|\le\bar{K}$$

Therefore, if $r(t)=\sup_{x,x_1\in Y}|r_x^{(0,1)}(t;x_1)|$, we have

$$|\frac{d}{dt}r(t)|\le\bar{K}r(t)$$

with $r(0)=1$, so that $|r_x^{(0,1)}(t;x_1)|\le r(t)\le e^{\bar{K}|t|}$.

With the notation $k=d(x,x_1)$ we claim that

$$|r_x^{(0,1)}(t;x_1)|\le\{e^{\bar{K}|t|}\}_k$$

where we have defined $\{e^u\}_k=e^u-\sum_{n=0}^{k-1}u^n/n!\le e^u\inf_{\ell\le k}u^\ell/\ell!$ For $k=0$ the claim has been proved above. For $k>0$ we have by induction

$$|\frac{d}{dt}r_x^{(0,1)}(t;x_1)|\le\bar{K}\{e^{\bar{K}|t|}\}_{k-1}$$

and our claim follows by integration, using $r_x^{(0,1)}(0,x_1)=0$.

Remember that $\sigma(x,x_1,\ldots,x_j)$ is the smallest length of a subgraph of Γ connecting $x,x_1,\ldots,x_j$. We claim that for $j\ge1$ there are constants $L_j>0$ and $M_j>0$ such that

$$|r_x^{(0,j)}(t;x_1,\ldots,x_j)|\le M_je^{j\bar{K}|t|}\inf_{0\le\tau\le\sigma}\frac{(L_j|t|)^\tau}{\tau!}\tag{1}$$

where $\sigma=\sigma(x,x_1,\ldots,x_j)$.

We have already proved (1) for $j=1$, with $L_1=\bar{K}$, $M_1=1$. For $j>0$ we have

$$\frac{d}{dt}r_x^{(0,j)}(t;x_1,\ldots,x_j)=\sum_{y\in B_x^1}\Phi_{xy}r_y^{(0,j)}(t;x_1,\ldots,x_j)+rest\tag{2}$$

The *rest* is a sum, over $y \in B^1_x$ and $\mathcal{X}$, of products of factors $r^{(0,j_n)}_{z_n}(t; X_n)$ where z_n is x or y, $\mathcal{X} = (X_n)$ is a partition of $(x_1, \ldots, x_j)$ into $|\mathcal{X}| > 1$ subsequences of length j_n, and each product has a coefficient which is a smooth function of q_x, q_y. Thus

$$|rest| \leq C_j \max_{\mathcal{X}} \exp(\sum_n j_n \bar{K}|t|) \prod_n \frac{(L_{j_n}|t|)^{\tau_n}}{\tau_n!} \leq C_j e^{j\bar{K}|t|} \frac{(L'_j|t|)^{\tau'}}{\tau'!}$$

where $L'_j = \max_{\mathcal{X}} \sum_n L_{j_n}$ and τ' must be of the form $\sum_n \tau_n$, *i.e.*, $0 \leq \tau' \leq \sum_n \sigma(z_n, X_n)$ where each z_n is either x or y, and therefore

$$\sum_n \sigma(z_n, X_n) + 1 \geq \sigma(x, x_1, \ldots, x_j) = \sigma$$

so that all values of τ' between 0 and $[\sigma - 1]_+$ are allowed. We have thus

$$|rest| \leq C_j e^{j\bar{K}|t|} \inf_{0 \leq \tau' \leq [\sigma-1]_+} \frac{(L'_j|t|)^{\tau'}}{\tau'!}$$

We shall prove (1) by induction on j, assuming now $j > 1$. First let us write

$$\sup_x |r^{(0,j)}_x(t; x_1, \ldots, x_j)| = r(t : x_1, \ldots, x_j) = e^{\bar{K}|t|} s(t)$$

and let

$$\sigma' = \sigma(x_1, \ldots, x_j) = \min_x \sigma(x, x_1, \ldots, x_j)$$

Then, for $0 \leq \tau' \leq [\sigma' - 1]_+$ and $t \geq 0$,

$$\frac{d}{dt} r(t; x_1, \ldots, x_j) \leq \bar{K} r(t; x_1, \ldots, x_j) + C_j e^{j\bar{K}t} \frac{(L'_j t)^{\tau'}}{\tau'!}$$

or

$$\frac{d}{dt} s(t) \leq C_j e^{(j-1)\bar{K}t} \frac{(L'_j t)^{\tau'}}{\tau'!}$$

Thus

$$\frac{ds}{dt} \leq \frac{d}{dt}[e^{(j-1)\bar{K}t} \frac{(C_j t)(L'_j t)^{\tau'}}{(\tau'+1)!}] \qquad \text{for} \qquad 0 \leq \tau' \leq \sigma' - 1$$

and also (taking $\tau' = 0$)

$$\frac{ds}{dt} \leq \frac{d}{dt} \frac{C_j}{(j-1)\bar{K}} e^{(j-1)\bar{K}t}$$

We shall take $L_j = L'_j + C_j$ and $M_j = 1 + C_j/L'_j + C_j[(j-1)\bar{K}]^{-1}$. In particular, we have

$$s(t) \leq M_j e^{(j-1)\bar{K}t} \frac{(L'_j t)^{\tau'+1}}{(\tau'+1)!} \qquad \text{for} \qquad 0 \leq \tau' \leq \sigma' - 1$$

$$s(t) \leq M_j e^{(j-1)\bar{K}t}$$

hence

$$s(t) \leq M_j e^{(j-1)\bar{K}t} \inf_{0\leq\tau\leq\sigma'} \frac{(L'_j t)^\tau}{\tau!}$$

and

$$|r_x^{(0,j)}(t : x_1, \ldots, x_j)| \leq M_j e^{j\bar{K}|t|} \inf_{0\leq\tau\leq\sigma'} \frac{(L'_j|t|)^\tau}{\tau!}$$

To prove (1), it suffices to show that if

$$\sigma(x, x_1, \ldots, x_j) \geq \sigma' + k$$

then

$$|r_x^{(0,j)}(t; x_1, \ldots, x_j)| \leq M_j e^{j\bar{K}|t|} \inf_{0\leq\tau\leq\sigma'+k} \frac{(L_j|t|)^\tau}{\tau!}$$

and we have just shown this for $k = 0$. We proceed now by induction on k for $k > 0$. For $y \in B_x^1$ we have

$$\sigma(y, x_1, \ldots, x_j) \geq \sigma(x, x_1, \ldots, x_j) - 1 \geq \sigma' + k - 1$$

Therefore, our induction asssumption and estimate of $|rest|$ give

$$|\frac{d}{dt} r_x^{(0,j)}(t; x_1, \ldots, x_j)| \leq \bar{K} M_j e^{j\bar{K}|t|} \inf_{0\leq\tau'\leq\sigma'+k-1} \frac{(L_j|t|)^{\tau'}}{\tau'!} + C_j e^{j\bar{K}|t|} \inf_{0\leq\tau'\leq\sigma'+k-1} \frac{(L'_j|t|)^{\tau'}}{\tau'!}$$

Since $L_j = L'_j + C_j \geq C_j + \bar{K}$, and $1 \leq M_j$, we may write for $t \geq 0$,

$$\frac{d}{dt} |r_x^{(0,j)}(t; x_1, \ldots, x_j)| \leq M_j e^{j\bar{K}|t|} \inf_{0\leq\tau'\leq\sigma'+k-1} L_j \frac{(L_j t)^{\tau'}}{\tau'!}$$

hence

$$|r_x^{(0,j)}(t; x_1, \ldots, x_j)| \leq M_j e^{j\bar{K}|t|} \frac{(L_j t)^\tau}{\tau!}$$

if $1 \leq \tau \leq \sigma' + k$, but the above inequality also holds by the induction assumption when $\tau = 0$, and this completes the proof of (1).

We discuss now the case $i > 0$. We have an explicit expression for $r^{(1,j)} = dr^{(0,j)}/dt$, given by the evolution equation for (p, q) if $j = 0$, by (2) if $j \geq 1$. We may differentiate repeatedly with respect to t, replacing the derivatives in the right-hand side by using either the evolution equation for (p, q) or (2). We express thus $r^{(i,j)}$ as a polynomial in the p_y and the $r_y^{(0,\ell)}$ with $\ell \leq j$, with coefficients that are smooth functions of the q_y. The indices y of the p_y, q_y, and $r_y^{(0,\ell)}$ that occur satisfy $d(x, y) \leq i$. Furthermore, in any given term of the polynomial, the factors $r_{y_1}^{(0,\ell_1)}(X_1), \ldots, r_{y_m}^{(0,\ell_m)}(X_m)$ that occur (with $(X_1, \ldots, X_m)$ forming a partition of $(x_1, \ldots, x_j)$) satisfy

$$\sigma(x, y_1, \ldots, y_m) \leq i$$

$$\sigma(x, y_1, \ldots, y_m) + \sigma(y_1, X_1) + \ldots + \sigma(y_m, X_m) \geq \sigma(x, x_1, \ldots, x_j) = \sigma$$

so that

$$\sigma(y_1, X_1) + \ldots + \sigma(y_m, X_m) \geq \sigma - i$$

Therefore, using (1), we see that $r^{(i,j)}$ is a polynomial of degree $\leq i$ in the p_y such that $y \in B_x^i$, with coefficients bounded in absolute value by

$$\text{const.} e^{j\bar{K}|t|} \inf_{0 \leq \tau \leq \sigma - i} \frac{(L_j|t|)^\tau}{\tau!}$$

if $i \leq \sigma$, otherwise by

$$\text{const.} e^{j\bar{K}|t|}$$

concluding the proof of the proposition. $\square$

A.2 (proof of Proposition 2.8).

Note that the conditions on the coefficients of $\mathcal{Q}$ are of the same form as those on the coefficients of $\mathcal{P}$ in Proposition 2.7, but σ has a new definition (and the L_j, M_{ij} may have to be chosen larger than for Proposition 2.7).

Note also that Lemma 2.1(b) gives, for $d(x, X) > 0$,

$$|\Delta r_x^{(0,0)}(t; X)| \leq \frac{(\bar{K}|t|)^\tau}{\tau!} \qquad \text{if} \qquad 1 \leq \tau \leq d(x, X)$$

Using also Lemma 2.1(a), this proves the Proposition in the case $(i, j) = (0, 0)$ since here $\sigma = d(x, X)$.

We shall later use the fact that for the q-component we have actually, for $d(x, X) \geq 0$,

$$|\Delta q_x(t; X)| = |q_x(t) - \tilde{q}_x(t)| \leq \frac{(\bar{K}|t|)^\tau}{\tau!} \qquad \text{if} \qquad 0 \leq \tau \leq d(x, X)$$

[this is because $q_x(t), \tilde{q}_x(t) \in \mathbf{T}$, so that $|q_x(t) - \tilde{q}_x(t)| \leq 1$].

In the study of $\Delta r_x^{(0,j)}$ for $j > 0$ we do not impose the condition $d(x, X) > 0$. If $j > 0$, we claim that there are constants $L_j > 0$ and $M_j > 0$ such that

$$|\Delta r_x^{(0,j)}(t; x_1, \ldots, x_j; X)| \leq M_j e^{j\bar{K}|t|} \inf_{0 \leq \tau \leq \sigma} \frac{(L_j|t|)^\tau}{\tau!} \tag{3}$$

where $\sigma = \sigma(x, x_1, \ldots, x_j; X)$.

This will be proved by induction on j, using (1) and the equation

$$\frac{d}{dt} \Delta r_x^{(0,j)}(t; x_1, \ldots, x_j; X) = \sum_{y \in B_x^1} \Phi_{xy}(q_x, q_y) \Delta r_y^{(0,j)}(t; x_1, \ldots, x_j; X) + rest$$

The *rest* here is a finite sum of products, each of which has exactly one factor with a Δ in front of it. The factors are: a coefficient depending smoothly on q_x, q_y, and factors $r_{z_n}^{(0,j_n)}$ where z_n is x or y and the X_n form a partition $\mathcal{X} = (X_n)$ of $(x_1, \ldots, x_j)$ into $|\mathcal{X}|$ subsequences of length j_n.

In particular, for $j = 1$, the *rest* is $\sum_y \Delta\Phi_{xy}.r_y^{(0,1)}$. Using the remark above on $|\Delta q_x|$, and the earlier bound on $|r_x^{(0,1)}|$ one finds

$$|rest| \leq \text{const.}\frac{(\bar{K}|t|)^k}{k!}.e^{\bar{K}|t|}\frac{(\bar{K}|t|)^\ell}{\ell!} \leq \text{const.}e^{\bar{K}|t|}\frac{(2\bar{K}|t|)^{k+\ell}}{(k+\ell)!}$$

where k is allowed values in $[0, d(y, X)]$ or $[0, d(x, X)]$ and ℓ is allowed values in $[0, d(y, x_1)]$, so that $k + \ell$ is allowed all values in $[0, [\sigma - 1]_+]$.

For general $j > 0$, using induction on j, and the bounds on $|\Delta q_x|, |r_x^{(0,j)}|$ shows that the products appearing in the *rest* have, in absolute value, bounds of the form

$$\text{const.}\frac{(\bar{K}|t|)^k}{k!}.(\exp\sum_n j_n\bar{K}|t|).\prod_n \frac{(L_{j_n}|t|)^{\ell_n}}{\ell_n!}$$

$$\leq \text{const.}e^{j\bar{K}|t|}\frac{[(\bar{K} + \sum_n L_{j_n})|t|]^{k+\sum \ell_n}}{(k + \sum \ell_n)!} \leq \text{const.}e^{j\bar{K}|t|}\frac{(L'_j|t|)^{\tau'}}{\tau'!}$$

where $L'_j = \bar{K} + \max_{\mathcal{X}} \sum_n L_{j_n}$, and we must now discuss the range of $\tau' = k + \sum \ell_n$. Remember that there is a Δ in front of one of the factors of the product we are considering.

If the Δ is in front of the coefficient depending smoothly on q_x, q_y, this corresponds to $k \in [0, d(z, X)]$ with $z = x$ or y, while $\ell_n \in [0, \sigma(z_n, X_n)]$ with $z_n = x$ or y. Since $d(x, y) = 1$, we have $d(z, X) + \sum_\ell \sigma(z_\ell, X_\ell) + 1 \geq \sigma(x, x_1, \ldots, x_j; X) = \sigma$; therefore $\tau' = k + \sum \ell_n$ is allowed all values such that $0 \leq \tau' \leq [\sigma - 1]_+$.

If the Δ is in front of one of the $r_{z_n}^{(0,j)}$, say for $n = a$, the corresponding ℓ_a is $\in [0, \sigma(z_a, X_a; X)]$ by the induction assumption, the other $r_{z_n}^{(0,j_n)}$ are $\in [0, \sigma(z_n, X_n)]$, and we have $k = 0$. Note that

$$\sigma(z_a, X_a; X) + \sum_{n \neq a} \sigma(z_n, X_n) + 1 \geq \sigma(x, x_1, \ldots, x_j; X) = \sigma$$

therefore $\tau' = \sum \ell_n$ is again allowed all values such that $0 \leq \tau' \leq [\sigma - 1]_+$. In conclusion we have

$$|rest| \leq C_j e^{j\bar{K}|t|} \inf_{0 \leq \tau' \leq [\sigma-1]_+} \frac{(L'_j|t|)^{\tau'}}{\tau'!}$$

To start the proof of (3) we write

$$\sup_x |\Delta_x^{(0,j)}(t; x_1, \ldots, x_j; X)| = r(t; x_1, \ldots, x_j; X) = e^{\bar{K}|t|}s(t)$$

and let $\sigma' = \sigma(x_1, \ldots, x_j; X) = \min_x \sigma(x, x_1, \ldots, x_j; X)$, Then for $\tau' \in [0, [\sigma' - 1]_+]$ and $t \geq 0$ we obtain, as in the proof of Proposition 2.7

$$\frac{d}{dt} s(t) \leq C_j e^{(j-1)\bar{K}t} \frac{(L'_j t)^{\tau'}}{\tau'!}$$

hence

$$|\Delta r_x^{(0,j)}(t; x_1, \ldots, x_j; X)| \leq M_j e^{j\bar{K}|t|} \inf_{0 \leq \tau \leq \sigma'} \frac{(L_j |t|)^\tau}{\tau!}$$

and the proof of (3) continues as the proof of (1).

The case $i > 0$ (taking now $d(x, X) > i$) is treated as in the proof of Proposition 2.7. ∎

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