

Stationary states of random Hamiltonian systems

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Summary. We investigate the ergodic properties of Hamiltonian systems subjected to local random, energy conserving perturbations. We prove for some cases, e.g. anharmonic crystals with random nearest neighbor exchanges (or independent random reflections) of velocities, that all translation invariant stationary states with finite entropy per unit volume are microcanonical Gibbs states. The results can be utilized in proving hydrodynamic behavior of such systems.

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1.1 Introduction

There has been much progress during the past ten years in deriving hydrodynamic type equations for a variety of microscopic model systems; for a review (see [Sp], [Fr4], [Y], [OVY]). A common feature of these models is the stochastic nature of their microscopic dynamics. This stochasticity plays a crucial role in various steps of the arguments leading from the microscopic evolution to the macroscopic one. It is therefore not clear just what are the requirements on particle systems evolving according to Hamiltonian dynamics to have the type of macroscopic behavior which are observed in nature, e.g. those described by the Euler equations.

Recently Yau [Y] and Olla, et al. [OVY] made some important progress in this direction. They managed to reduce the problem of proving the hydrodynamic limit in some cases, including Hamiltonian systems, to a reasonable, ergodicity type condition on the dynamics. Roughly speaking, they require that every “regular” translation invariant stationary state be of Gibbsian type. Regularity here means that the state has finite relative entropy (per unit volume) with respect to a Gibbs

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state. This requires in particular that the conditional distributions in any finite volume, Λ , given the configuration outside Λ , be absolutely continuous with respect to Lebesgue measure.

To prove such ergodicity for deterministic Hamiltonian systems is unfortunately still a formidable unsolved problem. Here too, the requirements on the Hamiltonian are far from understood at the present time (see [Si]) for a try at this task. To overcome this problem, [OVY] added a diffusive noise mimicking “randomizing collisions” between pairs of particles. This noise conserves momentum and energy, but otherwise uniformly spreads the relative momenta. It is sufficiently weak not to affect the hydrodynamic behavior on the time scale studied. To ensure that the system behaves ergodically, [OVY] require that the random force given by the noise is also acting between particles which are very far separated on a microscopic scale. Now it is clear that in real systems the effective (deterministic) randomness comes from the dynamics which are governed by local interactions. It is therefore interesting to investigate this ergodic problem for Hamiltonian systems with milder local random perturbations. Instead of diffusive forces, we consider randomized jumps, i.e. exchanges or reflections of velocities. In addition to its general interest in the hydrodynamic scaling limit, such local exchanges may be useful for computer simulation of hydrodynamic behavior.

Our approach to the problem goes back to Gallavotti and Verboven [GV]. They noticed that solutions to the stationary Liouville equation with Gaussian velocities are canonical Gibbs states. We show that this strong requirement can be replaced by weaker symmetry properties of the stationary state. In fact, exchangeability or reflection symmetry of the velocity distribution are sufficient to yield the desired result for regular translation invariant states of the Hamiltonian dynamics. The problem is therefore reduced to finding the minimal amount of local randomness which will force the stationary state to have the required symmetry. We investigate this problem here for a lattice system of coupled anharmonic oscillators. In this case the steps leading from the dynamics to the symmetry properties of the stationary state are simpler than for continuous particle systems. The results for the latter, which are currently proven only for the simplest type of Hamiltonian (ideal gas, see [ES]) will be described elsewhere; the part of the argument connecting symmetry with microcanonical Gibbs states remains unchanged.

1.2 The model

We consider a lattice system of coupled oscillators with self-potential U and symmetric nearest neighbor interaction V . Let $p_k \in \mathbb{R}$ and $q_k \in \mathbb{R}$ denote the velocity and the position of the oscillator at site $k \in \mathbb{Z}^d$. The formal Hamiltonian of the system can be written as

$$H = \sum_{k \in \mathbb{Z}^d} \left(\frac{1}{2} p_k^2 + U(q_k) + \frac{1}{2} \sum_{|j-k|=1} V(q_k - q_j) \right), \quad (1.1)$$

and the underlying evolution is defined by an infinite system of differential equations:

$$\dot{p}_k = -\frac{\partial H}{\partial q_k} = -U'(q_k) - \sum_{|j-k|=1} V'(q_k - q_j), \quad \dot{q}_k = p_k \text{ for } k \in \mathbb{Z}^d. \quad (1.2)$$

We now add to this Hamiltonian dynamics some "noise". This consists of random exchanges of velocities between neighboring sites. These take place independently at each bond of the lattice with a constant rate $a > 0$. The proof of desired ergodic properties for this combined dynamics, which clearly conserves energy, proceeds in several stages. First we show that every regular translation invariant stationary measure for this system is actually separately stationary under the exchanges and the Hamiltonian dynamics. The latter implies that it satisfies the time independent Liouville equation or in short it is "Liouville stationary" (LS). We then prove the general result that every LS measure which is exchangeable, i.e. which is symmetric in the velocities for arbitrary values of the position variables, must in fact be a microcanonical Gibbs measure. This means that the distribution of the configurations in a box Λ , given the configuration outside Λ , and the energy in Λ , is "uniform" on each energy shell, that is configurations with the same energy in Λ are equally likely. Therefore the infinite volume stationary measure is a superposition of Gibbs states with different temperatures. The derivation of the Gibbs property for an exchangeable LS measure uses its invariance with respect to the *infinite* group of translations of $\mathbb{Z}^d$. The existence of Gibbs states requires, of course, some conditions on U and V , which will be discussed in the next section.

In the case where the one body potential $U \equiv 0$, both the Hamiltonian evolution and the exchanges conserve momentum. We then obtain LS states which are superpositions of Gibbs states, defined now generally only on coordinate differences, with different temperatures and different parameters γ conjugate to the total momentum. In the case of an anharmonic chain, i.e. if $d=1$, the coordinate differences are independent with respect to a Gibbs state, thus the [OVY] methods can be applied to obtain Euler like equations for the conserved densities. Multi-dimensional models are more problematic because the coordinate differences are then subjected to constraints, thus the usual thermodynamic formalism is not available; we are going to discuss this question elsewhere.

We also consider the case where the random noise simply flips velocities, $p_k \rightarrow -p_k$, at random moments of time independently for all k . This mechanism violates the law of momentum conservation, and its stationary measures are symmetric with respect to reflection of the velocity at any site. To show that such reflection symmetric LS measures are microcanonical Gibbs states with vanishing mean velocities we need the presence of a *generic* interaction V between neighboring oscillators.

The outline of the rest of the paper is as follows. In Sect. 2 we give precise definitions of the random evolutions and summarize the main ideas and results. In Sects. 3 and 4 solutions of the time independent Liouville equation (LS) are shown to be superpositions of Gibbs states with different temperatures under various symmetry properties of the solution. Existence and regularity of the random evolutions are proven in Sect. 5. Then the proofs of the main results are completed in Sect. 6 by using an entropy argument implying that translation invariant stationary states of the random evolutions satisfy (LS) and the symmetry conditions under which we have solved (LS) before.

2 Mathematical formulation and main results

For convenience we assume that U and V are non-negative with bounded second derivatives. Then the infinite system of Hamiltonian equations (1.2) has uniquely

defined global solutions for each initial configuration of subexponential growth. More exactly, let Ω denote the set of configurations $\omega = (p_k, q_k)_{k \in \mathbb{Z}^d}$ such that $\|\omega\|_\alpha < +\infty$ for each $\alpha > 0$, where

$$\|\omega\|_\alpha^2 = \sum_{k \in \mathbb{Z}^d} e^{-\alpha|k|} [p_k^2 + q_k^2]. \quad (2.1)$$

We equip Ω with its natural product topology and Borel field $\mathcal{A}$, the set of Borel probabilities will be denoted by $\mathcal{P}(\Omega)$. The space of continuous and bounded cylinder functions $\varphi: \Omega \rightarrow \mathbb{R}$ will be denoted by $\mathbf{C}_0(\Omega)$, while $\mathbf{C}_0^k(\Omega)$ is the set of $\varphi \in \mathbf{C}_0(\Omega)$ having k continuous and bounded partial derivatives. If $\mathcal{B} \subset \mathcal{A}$ is a σ -field, then $\varphi \in \mathcal{B}$ indicates that φ is measurable with respect to $\mathcal{B}$ and if $\mathcal{B}$ is generated by some measurable map ψ , then $\mu[\varphi|\psi] \equiv \mu[\varphi|\mathcal{B}]$ denotes the conditional expectation of φ . Let A be a subset of $\mathbb{Z}^d$, its complementary set is denoted as A^c and ∂A is the boundary of A , that is the set of $j \notin A$ having a neighbor $k \in A$. The variables $\omega_A := (p_k, q_k)_{k \in A}$ generate a σ -field $\mathcal{A}_A$; $p_A := (p_k)_{k \in A}$, $q_A := (q_k)_{k \in A}$, and the notation $\omega_A = (\omega_A | \omega_B)$ is also used when $A = A \cup B$ and $A \cap B = \emptyset$.

Since U' and V' are uniformly Lipschitz continuous, the most standard iteration procedure yields existence of uniquely defined global solutions in Ω (see [LLL], [Fr1], [SS]). This flow is generated by the Liouville operator, $\mathcal{L}$,

$$\mathcal{L} = \sum_{k \in \mathbb{Z}^d} \mathcal{L}_k, \quad \mathcal{L}_k \varphi = p_k \frac{\partial \varphi}{\partial q_k} - \frac{\partial H}{\partial q_k} \frac{\partial \varphi}{\partial p_k} \text{ if } \varphi \in \mathbf{C}_0^1(\Omega). \quad (2.2)$$

Stationary states of Hamiltonian dynamics are characterized by the so-called stationary Liouville equation:

$$\int \mathcal{L} \varphi(\omega) \mu(d\omega) = 0 \quad \text{for } \varphi \in \mathbf{C}_0^1(\Omega). \quad (\text{LS})$$

To give a meaning to this equation, we assume that μ satisfies the following moment condition:

$$\int \left(|p_k| + \left| \frac{\partial H}{\partial q_k} \right| \right) d\mu < +\infty \text{ for each } k \in \mathbb{Z}^d. \quad (2.3)$$

It is well known that Gibbs states and their superpositions are stationary states of Hamiltonian dynamics. Gibbs states are defined in terms of H_A , which is defined for any finite $A \in \mathbb{Z}^d$ and $\omega \in \Omega$ by

$$\begin{aligned} H_A(\omega) &\equiv H_A(\omega_A | \omega_{\partial A}) := H_A^0(\omega) + \sum_{k \in A} \sum_{\substack{j \in A^c \\ |j-k|=1}} V(q_k - q_j), \\ H_A^0(\omega) &\equiv H_A^0(\omega_A) := \sum_{k \in A} \left(\frac{1}{2} p_k^2 + U(q_k) + \frac{1}{2} \sum_{\substack{j \in A \\ |j-k|=1}} V(q_k - q_j) \right). \end{aligned} \quad (2.4)$$

Definition 2.1 A probability measure $\mu \in \mathcal{P}(\Omega)$ is called a Gibbs state for H with inverse temperature $\beta > 0$ if its conditional distributions are specified as $\mu[d\omega_A | \omega_{A^c}] = \lambda_{\beta, A}[d\omega_A]$ μ -a.s. for each finite $A \subset \mathbb{Z}^d$, where

$$\lambda_{\beta, A}[d\omega_A | \omega_{\partial A}] := \frac{1}{Z_A(\beta, \omega_{\partial A})} \exp[-\beta H_A(\omega_A | \omega_{\partial A})] d\omega_A,$$

and Z_A is the normalization.

Since U and V are non-negative, the following simple condition is sufficient for the finiteness of Z_A at any inverse temperature $0 < \beta < \infty$:

$$\int_{-\infty}^{+\infty} \exp[-\beta U(x)] dx < +\infty \quad \text{for all } \beta > 0. \quad (2.5)$$

Let us remark that under (2.5), Gibbs states can be constructed for all $\beta > 0$ as the limit of finite volume Gibbs distributions with periodic boundary conditions on the product space $(\mathbb{R} \times \mathbb{R})^{\mathbb{Z}^d}$. Moreover, if $\lim_{|x| \rightarrow +\infty} |x| \exp(-\beta U(x)) = 0$ for all $\beta > 0$ as $|x| \rightarrow +\infty$, then our configuration space Ω is of full measure with respect to such limiting Gibbs states. Nevertheless, we *do not need* at all the existence of any Gibbs state for H in this paper. Under a bit stronger condition on the growth of U the entropy argument of Sect. 6 yields existence of stationary states for a wide class of stochastic dynamics, whence the existence of Gibbs states and the equivalence of ensembles also follows from the results below.

All superpositions of Gibbs states with different temperatures are microcanonical states in the following sense.

Definition 2.2 *A microcanonical Gibbs state with a fixed energy constraint is a Borel probability $\mu \in \mathcal{P}(\Omega)$ specified by $\mu[d\omega_A | \omega_{A^c}, H_A] = \lambda_{\beta, A}[d\omega_A | \omega_{\partial A}, H_A]$ μ -a.s. for each finite $A \subset \mathbb{Z}^d$.*

Notice that $\lambda_{\beta, A}[d\omega_A | \omega_{\partial A}, H_A]$ is just the normalized surface measure (uniform distribution) on the corresponding energy shell $\mathcal{E}$, see (3.11). Under fairly general conditions, every microcanonical Gibbs state is a stationary measure of Hamiltonian dynamics, but a rigorous proof of the converse statement seems to be extremely hard. Simple and more sophisticated examples show that it is even not true without some additional conditions. Indeed, if we choose the initial configuration such that $p_k = p_0$ and $q_k = q_0$ for each k , then the resulting periodic orbits carry some stationary states, which are certainly not microcanonical Gibbs. Of course, such degeneracies are ruled out by local absolute continuity of the stationary state, but periodic initial configurations might yield even more complex, locally absolutely continuous stationary measures via KAM theory (see [A]) with further references. It is also known that harmonic oscillators have additional, and fairly regular stationary states [LS]. This is the reason why we introduce additional symmetries corresponding to randomized versions of classical dynamics.

The following exchange symmetry (ES) of the velocity distribution is sufficient to solve (LS):

$$\int \mathcal{G}_{k,j}^E \varphi d\mu = 0; \quad \mathcal{G}_{k,j}^E \varphi(\omega) := \varphi(\omega^{k,j}) - \varphi(\omega) \quad \text{for } \varphi \in C_0(\Omega), |j-k|=1, \quad (\text{ES})$$

where $\omega^{k,j}$ is obtained from ω by exchanging p_k and p_j . In the next section we show that (ES) implies the conditional independence of velocities and positions, given $\mathcal{A}_{\text{inv}}$, the field of translation invariant events. Moreover, (LS) and (ES) yield some $\beta \in \mathcal{A}_{\text{inv}}$ such that almost every realization of $\mu[d\omega | \mathcal{A}_{\text{inv}}]$ is a Gibbs state with the corresponding β as its inverse temperature, that is we have a statement on the equivalence of ensembles, cf. [G]. The only condition we need is that our measure is non-degenerate in the following sense.

Definition 2.3 *We say that a state $\mu \in \mathcal{P}(\Omega)$ is disordered if*

$$\mu[p_k | \mathcal{A}_{\text{tail}}]^2 < \mu[p_k^2 | \mathcal{A}_{\text{tail}}] < \infty \quad \mu\text{-a.s. for each } k \in \mathbb{Z}^d,$$

where $\mathcal{A}_{\text{tail}}$ is the tail field of Ω .

Let us remark that the periodic stationary states mentioned above are not disordered, and in the first counter-example even the random exchange mechanism preserves the stationary state.

Theorem 2.1 *Suppose that μ is translation invariant. Then (ES) implies the conditional independence of velocities and positions given $\mathcal{A}_{inv}$, i.e. $\mu[dp|q, \mathcal{A}_{inv}] = \mu[dp|\mathcal{A}_{inv}]$. Moreover, if μ is a disordered state, then (ES) and (LS) imply the existence of a translation invariant and μ -a.s. positive random variable, β , such that almost every realization of $\mu[d\omega|\mathcal{A}_{inv}]$ is a Gibbs state with inverse temperature β ; therefore μ is a microcanonical Gibbs state.*

The next symmetry property (RS) is related to random reflections of velocities:

$$\int \mathcal{G}_k^R \varphi d\mu = 0; \quad \mathcal{G}_k^R \varphi(\omega) := \varphi(\omega^k) - \varphi(\omega) \quad \text{for } \varphi \in C_0(\Omega), \quad (\text{RS})$$

and ω^k is obtained from $\omega = (p_k, q_k)_{k \in \mathbb{Z}^d}$ by replacing p_k by $-p_k$, other coordinates remain unchanged. In this case we need additional regularity conditions.

Theorem 2.2 *Let U and V be infinitely differentiable, and suppose that $V''(x) = 0$ implies $V'''(x) \neq 0$ for each $x \in \mathbb{R}$. If $\mu \in \mathcal{P}(\Omega)$ is locally absolutely continuous, then (LS) and (RS) imply (ES). Therefore if μ is also disordered and translation invariant, then it is a microcanonical Gibbs state.*

We turn now to the construction of random evolutions. We consider modified evolutions generated by $\mathcal{G} = \mathcal{L} + a\mathcal{G}_{ran}$, where $a > 0$ and $\mathcal{G}_{ran}$ describes random effects. Random reflections correspond to $\mathcal{G}_{ran} = \mathcal{G}^R$, while random exchanges are generated by $\mathcal{G}_{ran} = \mathcal{G}^E$, where

$$\mathcal{G}^R = \sum_{k \in \mathbb{Z}^d} \mathcal{G}_k^R, \quad \mathcal{G}^E = \frac{1}{2} \sum_{k \in \mathbb{Z}^d} \sum_{|j-k|=1} \mathcal{G}_{k,j}^E. \quad (2.6)$$

The associated random evolutions are defined as solutions to the integral equations (5.1) and (5.2), respectively.

Theorem 2.3 *Suppose that U'' and V'' are bounded, and let $\mathcal{G} = \mathcal{L} + a\mathcal{G}^E$ or $\mathcal{G} = \mathcal{L} + a\mathcal{G}^R$, where $a > 0$. Then there exists a Markov process, $\mathcal{P}^t$ with phase space Ω such that the forward Kolmogorov equation holds true in the following form. If $\mu \in \mathcal{P}(\Omega)$ and $\int \|\omega\|_\alpha^2 d\mu < \infty$ for some $\alpha > 0$, then $\int \|\omega\|_\alpha^2 d\mu_t$ stays finite for all $t > 0$ and*

$$\int \varphi d\mu_t = \int \varphi d\mu + \int_0^t ds \int \mathcal{G} \varphi d\mu_s \quad \text{for } \varphi \in C_0^1(\Omega),$$

where $\mu_t = \mu \mathcal{P}^t$, $t \geq 0$ denotes the state of the process with initial distribution μ . Stationary states satisfying the moment condition (2.3) are characterized by the stationary Kolmogorov equation:

$$\int \mathcal{G} \varphi(\omega) \mu(d\omega) = 0 \quad \text{for } \varphi \in C_0^1(\Omega). \quad (\text{SK})$$

The derivation of the symmetry properties we used in solving the stationary Liouville equation is based on the notion of relative entropy; this is the point where we exploit the existence and regularity properties of randomized evolutions. As a family of reference measures we use finite volume Gibbs states λ_n^0 with free boundary conditions. More exactly, let $\Lambda_n \equiv [-n, +n]^d \cap \mathbb{Z}^d$, $n = 0, 1, \dots$ denote

a distinguished sequence of cubic boxes, then λ_n^0 is a probability measure on $\mathcal{A}_n \equiv \mathcal{A}_{\Lambda_n}$ such that

$$d\lambda_n^0 = \exp[-H_{\Lambda_n}^0(\omega_{\Lambda_n}) - F_n^0] d\omega_{\Lambda_n}, \quad F_n^0 := \log \int \exp[-H_{\Lambda_n}^0(\omega_{\Lambda_n})] d\omega_{\Lambda_n}. \quad (2.7)$$

Definition 2.4 Let μ and λ be probability measures on the σ -field $\mathcal{B}$, then the entropy of μ , relative to λ is defined as

$$I_{\mathcal{B}}[\mu|\lambda] = \sup_{h \in \mathcal{B}} \left\{ \int h d\mu - \log \int e^h d\lambda : \int e^h d\lambda < +\infty \right\}.$$

If $\mu \in \mathcal{P}(\Omega)$, $\lambda = \lambda_n^0$ and $\mathcal{B} = \mathcal{A}_n$ then the notation $I_n[\mu] \equiv I_{\mathcal{A}_n}[\mu|\lambda_n^0]$ is used, and

$$\limsup_{n \rightarrow +\infty} (1+2n)^{-d} I_n[\mu] := \bar{I}[\mu]$$

is the relative entropy of μ per unit volume. Let $\mathcal{P}_0(\Omega)$ denote the set of translation invariant $\mu \in \mathcal{P}(\Omega)$ such that $\bar{I}[\mu] < +\infty$.

It is easy to check that $I_n[\mu] < +\infty$ implies that $\mu_n \ll \lambda_n^0$ and $I_n[\mu] = \int \log f_n d\mu$, where $f_n = d\mu_n/d\lambda_n^0$ and μ_n denotes the restriction of μ to $\mathcal{A}_n$. Observe that if I_n is finite then its definition yields an explicit bound for $\int H_{\Lambda_n}^0 d\mu$. Since $V \geq 0$, by the usual subadditivity argument (cf. [R]), it follows that the limit below exists and

$$\bar{F}^0 := \inf_n (2n+1)^{-d} F_n^0 = \lim_{n \rightarrow \infty} (2n+1)^{-d} F_n^0.$$

Therefore if μ is translation invariant then the sequence $(1+2n)^{-d} I_n[\mu]$ converges to $\bar{I}[\mu]$ as $n \rightarrow +\infty$, and $\bar{I}$ is a convex and lower semicontinuous function of $\mu \in \mathcal{P}_0(\Omega)$ with respect to the weak convergence of probability measures. We are looking for solutions to (SK) within the class $\mathcal{P}_0(\Omega)$ of probability measures. To control entropy of the evolved state, the following stability condition will be assumed. We have some constant K such that

$$|V'(x-y)|^2 \leq K[1 + V(x-y) + U(x) + U(y)] \quad \text{for each } x, y \in \mathbb{R}. \quad (2.8)$$

In addition to (2.8) we suppose that

$$|U'(x)| \leq K[1 + U(x)] \quad \text{for each } x \in \mathbb{R}, \quad (2.9)$$

then $\mu \in \mathcal{P}_0(\Omega)$ implies (2.3). In the following theorems the boundedness of U'' and V'' and conditions (2.5), (2.8), (2.9) are assumed.

Theorem 2.4 Suppose that $\mu \in \mathcal{P}_0(\Omega)$ is a disordered stationary measure of the dynamics with random exchanges, then μ satisfies (LS) and (ES), thus it is a microcanonical Gibbs state.

In the case of reflections we have:

Theorem 2.5 Suppose that U and V are infinitely differentiable, and $V''(x) = 0$ implies $V'''(x) \neq 0$ for each $x \in \mathbb{R}$. If $\mu \in \mathcal{P}_0(\Omega)$ is a disordered stationary state of the dynamics with random reflections of velocities, then μ satisfies (LS) and (RS), thus μ is a microcanonical Gibbs state.

The derivation of symmetry properties (ES) and (RS) for stationary states of the random evolutions is based on an entropy argument that goes back to [Ho]. The

main steps can be outlined as follows, proofs are postponed to Sect. 6. Since Hamiltonian evolution does not contribute to entropy production, the temporal derivative of the relative entropy at a stationary state can formally be written as

$$\dot{I}_n = \int \mathcal{G} \log f_n d\mu = -aD_n[\mu] + B_n[\mu] = 0, \quad (2.10)$$

where B_n is a boundary term, while D_n is the essential, volume term of entropy production due to random effects.

The volume term of entropy production caused by exchange of velocities is

$$D_n = D_n^E[\mu] := \frac{1}{2} \sum_{k \in \Lambda_n} \sum_{\substack{j \in \Lambda_n \\ |j-k|=1}} \int \log \frac{f_n(\omega)}{f_n(\omega^{k,j})} \mu(d\omega). \quad (2.11)$$

In the case of velocity reflections we have

$$D_n = D_n^R[\mu] := \sum_{k \in \Lambda_n} \int \log \frac{f_n(\omega)}{f_n(\omega^k)} \mu(d\omega). \quad (2.12)$$

The boundary terms B_n will be specified and estimated in the last section. Since μ is translation invariant by assumption, we have $D_n \approx n^d$ while $B_n \approx n^{d-1}$, thus from (2.12) we get $D_n[\mu] = 0$ for each n . Each term of D_n is again a relative entropy, which is non-negative and vanishes only if the related distributions coincide. Therefore we have (RS) and (ES), respectively, thus (SK) implies (LS), too.

Partial information of this kind on the structure (symmetry) of our stationary measure μ can now be fed back into the stationary Liouville equation, that is we have to solve (LS) under some additional symmetry property. In this way the problem can be reduced to KMS type conditions, which admit an easy solution, at least if the state is a disordered one.

3 Symmetric solutions to the stationary Liouville equation

In this section we initiate a systematic study of symmetry properties of probability measures that are useful in solving (LS). Gibbs states admit a nice characterization in terms of integration by parts, namely every Gibbs state with inverse temperature $\beta > 0$ satisfies

$$\int \frac{1}{\beta} \frac{\partial \varphi}{\partial p_k} d\mu = \int \varphi p_k d\mu \text{ for } \varphi \in C_0^1(\Omega), \quad k \in \mathbb{Z}^d \text{ if } \varphi p_k \in C_0(\Omega) \quad (\text{KMSP})$$

and

$$\int \frac{1}{\beta} \frac{\partial \varphi}{\partial q_k} d\mu = \int \varphi \frac{\partial H}{\partial q_k} d\mu \text{ for } \varphi \in C_0^1(\Omega), \quad k \in \mathbb{Z}^d \text{ if } \varphi \partial_k H \in C_0(\Omega), \quad (\text{KMSQ})$$

where $\partial_k H = \partial H / \partial q_k$, and the converse statement is also true, see Theorem 3.1. On the other hand, (KMSQ) and (KMSP) imply (LS) under (2.3).

An integration by parts formula for microcanonical Gibbs states is the following identity:

$$\int \mathcal{L}_k \varphi d\mu = 0 \quad \text{for } k \in \mathbb{Z}^d \text{ and } \varphi \in C_0^1(\Omega). \quad (\text{MIP})$$

Let us remark that (MIP) does make sense even for a general $\mu \in \mathcal{P}(\Omega)$ because here the boundedness of φp_k and $\varphi \partial_k H$ may be assumed without any confusion. We shall show later that (MIP) yields a differential characterization of microcanonical states.

It is easy to check that (KMSP) and (KMSQ) together are equivalent to the classical KMS condition [GV], and each is implied by reversibility of μ with respect to the generators $\mathcal{G}_{k,\beta}^P$ and $\mathcal{G}_{k,\beta}^Q$, respectively, where

$$\begin{aligned}\mathcal{G}_{k,\beta}^P \varphi &= \frac{1}{\beta} \frac{\partial^2 \varphi}{\partial p_k^2} - \frac{\partial \varphi}{\partial p_k} p_k \quad \text{for } \varphi \in C_0^2(\Omega), \\ \mathcal{G}_{k,\beta}^Q \varphi &= \frac{1}{\beta} \frac{\partial^2 \varphi}{\partial q_k^2} - \frac{\partial \varphi}{\partial p_k} \frac{\partial H}{\partial q_k} \quad \text{for } \varphi \in C_0^2(\Omega).\end{aligned}\quad (3.1)$$

Remark 3.1 Since (KMSP) and (KMSQ) are statements on the local specifications of μ , in all results where (LS) has not been assumed, we can replace β by a tail-measurable function, provided that it is positive μ -a.s.

Now we show that the (KMSP) and (KMSQ) conditions are equivalent to the DLR equations, which is the definition of Gibbs states. In view of the decomposition $d\omega_A = dp_A dq_A$, symbols like $\mu[dp_A | \omega_{A^c}]$ or $\lambda_{\beta,A}[dq_A | q_{\partial A}]$ refer to the corresponding conditional marginal distributions.

Theorem 3.1 (KMSP) implies $\mu[dp_A | p_{A^c}, q] = \lambda_{\beta,A}[dp_A] \mu$ -a.s., while (KMSQ) implies $\mu[dq_A | \omega_{A^c}, p] = \lambda_{\beta,A}[dq_A | q_{\partial A}] \mu$ -a.s. for each finite $A \subset \mathbb{Z}^d$, and either of them together with (LS) imply that μ is a Gibbs state with inverse temperature β .

Proof. Let $\psi_A(\omega) = \exp[\beta H_A(\omega)]$ and introduce a σ -finite measure μ_A by $d\mu_A = \frac{1}{\beta} \psi_A d\mu$, then from (KMSP) or from (KMSQ) with $\varphi = \psi \psi_A$ we obtain that

$$\int \frac{\partial \psi}{\partial p_k} d\mu_A = 0 \quad \text{or} \quad \int \frac{\partial \psi}{\partial q_k} d\mu_A = 0 \quad \text{for } k \in A \text{ and } \psi \in C_0^1(\Omega), \quad (3.2)$$

respectively. Because of integrability problems, we have to assume first that ψ has compact support, the general case follows then by continuity. Since (3.2) is a differential characterization of Lebesgue measure dp_A or dq_A , we see in both cases that almost every projection of μ_A on $\mathbb{R}^A$ is invariant under Euclidean translations, which completes the proof of the first statement.

Suppose now (KMSP) and (LS), and let $\varphi(\omega) = \psi(q) p_j$, where $\psi \in C_0^1(\Omega)$. From the first statement we know already that $\mu(d\omega) = \mu(dp) \mu(dq)$ and the velocities are independent Gaussian variables, thus from (LS)

$$\int \psi(q) \frac{\partial H}{\partial q_j} d\mu = \sum_{k \in \mathbb{Z}^d} \int \frac{\partial \psi}{\partial q_k} p_k p_j d\mu = \int \frac{1}{\beta} \frac{\partial \psi}{\partial q_j} d\mu,$$

which is just (KMSQ) for functions depending only on the q -coordinates. Using $\tilde{\psi}_A = \exp(\beta \tilde{H}_A(q))$ instead of ψ_A , where

$$\tilde{H}_A(q) = H_A(\omega) - \sum_{k \in A} \frac{1}{2} p_k^2,$$

and substituting $\varphi(q) = \psi(q) \tilde{\psi}_A$, in the same way as before we obtain that $\mu[dq_A | q_{A^c}] = \lambda_{\beta,A}[dq_A | q_{\partial A}] \mu$ -a.s., thus we have a full description of the local

specifications of μ . The case of (LS) and (KMSQ) is almost the same, then we choose our test function as $\varphi = \psi(p)q_k$. $\square$

(ES) and (LS) reduce to the KMS conditions as follows.

Proof of Theorem 2.1 First we prove the conditional independence of velocities and positions given $\mathcal{A}_{inv}$, the field of invariant events. Let $\varphi_0, \psi_0 \in C_0(\Omega)$ be such that φ_0 depends only on velocities, while ψ_0 depends only on positions, and let φ_k and ψ_k denote their translates by $k \in \Omega$. This means that if $p = (p_j)_{j \in \mathbb{Z}^d}$, $q = (q_j)_{j \in \mathbb{Z}^d}$ then $\varphi_k(p) = \varphi_0((p_{j-k})_{j \in \mathbb{Z}^d})$ and $\psi_k(q) = \psi_0((q_{j-k})_{j \in \mathbb{Z}^d})$. Then we have

$$\int \varphi_k(p) \psi_0(q) d\mu = \int \varphi_0(p) \psi_0(q) d\mu = \int \varphi_k(p) \psi_k(q) d\mu, \quad (3.3)$$

where the first equality follows from (ES), while the second one is a consequence of the translation invariance of μ . Therefore, if $\chi_k(q) = \mu[\varphi_k | q]$ denotes the conditional expectation of φ_k given q , then χ_k does not depend on k , and it turns out to be a translation invariant, i.e. an $\mathcal{A}_{inv}$ -measurable function. Since φ_0 and ψ_0 are arbitrary cylinder functions, this implies the conditional independence of velocities and positions given $\mathcal{A}_{inv}$.

Now we can identify the distribution of positions as follows. Let $u(q) = \mu[p_k | \mathcal{A}_{inv}]$ and define $\beta = \beta(q)$ by $\beta^{-1} + u^2 = \mu[p_k^2 | \mathcal{A}_{inv}]$. In view of our previous observation, they do not depend on k . Now we put $\psi = \varphi(q)(p_j - u)$. Since u is tail measurable, (LS) results in

$$\int \varphi \frac{\partial H}{\partial q_j} d\mu = \int \frac{1}{\beta} \frac{\partial \varphi}{\partial q_j} d\mu + \sum_{k \neq j} \int (p_k p_j - u^2) \frac{\partial \varphi}{\partial q_k} d\mu. \quad (3.4)$$

On the other hand, if $j \neq k$ and $i \neq k$, then from (ES)

$$\int \psi(q) p_k p_j d\mu = \int \psi(q) p_k p_i d\mu = \int \psi(q) p_k \frac{1}{|A|} \sum_{i \in A} p_i d\mu \quad (3.5)$$

whenever $k \notin A$, thus the Ergodic Theorem implies $\mu[p_k p_j | \mathcal{A}_{inv}] = u^2(q)$ whenever $k \neq j$, that is the sum on the right hand side of (3.4) vanishes. This means that we have a (KMSQ) characterization of the distribution of positions, it turns out to be a mixture of Gibbs states with random temperature, see the proof of Theorem 3.1.

Now we can feed back this information into the stationary Liouville equation to conclude Theorem 2.1. We choose our test function as $\phi_j = \phi(p)q_j$ and exploit the conditional independence of the velocities and positions. From (LS) and (KMSQ) for functions depending only on positions we get

$$\int \phi(p) p_j d\mu = \sum_{k \in \mathbb{Z}^d} \int q_j \frac{\partial \phi}{\partial p_k} \frac{\partial H}{\partial q_k} d\mu = \int \frac{1}{\beta} \frac{\partial \phi(p)}{\partial p_j} d\mu, \quad (3.6)$$

which is just (KMSP) for $\phi = \phi(p)$, and completes the proof by applying the previous argument to the ergodic components $\mu[dq | \mathcal{A}_{inv}]$ of the joint distribution $\mu[dq]$ of positions. $\square$

Although (MIP) has no direct characterization in terms of reversibility of $\mathcal{G}_k^R$, cf. (3.1), it is related to random reflections of velocities via (LS) as follows.

Theorem 3.2 (RS) and (LS) imply (MIP).

Proof. In view of (LS)

$$\sum_{k \in \mathbb{Z}^d} \int \frac{\partial \varphi}{\partial q_k} p_k d\mu = \sum_{k \in \mathbb{Z}^d} \int \frac{\partial \varphi}{\partial p_k} \frac{\partial H}{\partial q_k} d\mu \quad \text{for } \varphi \in \mathbf{C}_0^1(\Omega). \quad (3.7)$$

Let $\mathbf{C}_0^*(\Omega)$ denote the space of $\varphi \in \mathbf{C}_0(\Omega)$ such that either $\varphi(\omega^k) = \varphi(\omega)$ for $\omega \in \Omega$, or $\varphi(\omega^k) = -\varphi(\omega)$ for each $\omega \in \Omega$; the set of $k \in \mathbb{Z}^d$ satisfying the second relation will be denoted by $\Lambda(\varphi) \subset \mathbb{Z}^d$. If $\varphi \in \mathbf{C}_0^*(\Omega)$ is continuously differentiable, then both $\psi_k = \partial \varphi / \partial p_k$ and $\psi_k^\circ = \partial \varphi / \partial q_k$ belong to $\mathbf{C}_0^*(\Omega)$, moreover $\Lambda(\psi_k) = \Lambda(\varphi) \setminus \{k\}$ if $k \in \Lambda(\varphi)$, $\Lambda(\psi_k) = \Lambda(\varphi) \cup \{k\}$ if $k \notin \Lambda(\varphi)$, while $\Lambda(\psi_k^\circ) = \Lambda(\varphi)$ for all $k \in \mathbb{Z}^d$. Since (RS) implies $\int \varphi d\mu = 0$ if $\varphi \in \mathbf{C}_0^*(\Omega)$ and $\Lambda(\varphi) \neq \emptyset$, we have

$$\int \frac{\partial \varphi}{\partial q_k} p_k d\mu = \int \frac{\partial \varphi}{\partial p_k} \frac{\partial H}{\partial q_k} d\mu = 0 \quad \text{unless } \Lambda(\varphi) = \{k\}, \quad (3.8)$$

thus comparing (3.7) and (3.8) we get (MIP) for $\varphi \in \mathbf{C}_0^*(\Omega)$. On the other hand, as any $\varphi \in \mathbf{C}_0^1(\Omega)$ decomposes into a finite sum of continuously differentiable functions from $\mathbf{C}_0^*$, thus we have (MIP) for all $\varphi \in \mathbf{C}_0^1(\Omega)$. $\square$

Our next observation is that (MIC) yields a differential characterization of the surface measure of energy shells, cf. (KMSP), (KMSQ) and (3.2). Suppose first that μ admits smooth local densities $f_A = \mu[d\omega_A]/d\omega_A$, then (MIP) turns into

$$\frac{\partial f_A}{\partial p_k} \frac{\partial H}{\partial q_k} = \frac{\partial f_A}{\partial q_k} p_k \quad \text{for } k \in \Lambda \quad (3.9)$$

and for each finite $\Lambda \subset \mathbb{Z}^d$. The characteristics of this system are trajectories solving

$$p_k dp_k + \frac{\partial H}{\partial q_k} dq_k = 0. \quad (3.10)$$

Therefore if we show that any pair of points on each energy shell $H_A = \text{const}$ can be connected by a finite chain of characteristics, then the continuity of f_A would imply that it is constant on the components of the energy shell. On the other hand, an energy shell may not be topologically connected if H_A is not convex, thus we are faced with two difficulties.

The problem of existence of smooth local densities can be solved as follows. Let $\mathcal{E}$ denote the energy shell,

$$\mathcal{E}(e, \omega_{A^c}) \equiv \mathcal{E}(e, \omega_{\partial A}) := \{\omega_A \in (\mathbb{R} \times \mathbb{R})^A; H_A(\omega_A | \omega_{\partial A}) = e\} \quad (3.11)$$

and denote L^k the restriction of $\mathcal{L}_k$ to this surface. Then the operator G ,

$$G = \frac{1}{2} \sum_{k \in \Lambda} (L^k)^2 \quad (3.12)$$

is a hypoelliptic one, thus by Hörmander's theorem (see e.g. [IK], [K]), G generates smooth diffusions on each component of the energy surface. Since this diffusion, like the flow generated by any L^k , preserves both the surface measure and the projection of μ on the energy shell, the latter admits a smooth density, thus the previous argument applies. A first consequence of (MIP) and (LS) is the following.

Theorem 3.3 *Suppose that U and V are infinitely differentiable, and $V''(x) = 0$ implies $V'''(x) \neq 0$ for each $x \in \mathbb{R}$. If $\mu \in \mathcal{P}(\Omega)$ is locally absolutely continuous, and satisfies*

(MIP), then its projection on almost every energy shell admits an infinitely differentiable density with respect to the surface measure of the energy shell, and the density is constant on each component of $\mathcal{E}(e, \omega_{A^c})$.

Remark 3.2 The technical condition that $V''=0$ implies $V''' \neq 0$ can be relaxed to the following one. For each $x \in \mathbb{R}$ there exists an $n \geq 2$ such that $V^{(n)}(x) \neq 0$.

Because of its technical nature, we postpone the proof of Theorem 3.3 to the next section. Of course, the energy shell is connected if both U and V are convex; then we have nothing more to do. Otherwise we conclude first (ES), whence Theorem 2.2 follows from Theorem 3.3 by Theorem 2.1.

Corollary 3.1 *Under conditions of Theorem 3.3, (MIP) implies (ES).*

Proof. To conclude the statement, it is enough to note that $\omega_A^{k,j}$ and ω_A belong to the same component whenever $k, j \in A$, thus even the conditional distributions $\mu[d\omega_A | \omega_{A^c}, H_A]$ satisfy (ES). $\square$

4 The energy shell

This section is devoted to an application of Hörmander's theorem and controllability theory of ordinary differential equations (see [E] and [He]). The proof of Theorem 3.3 is based on a series of lemmas.

Lemma 4.1 *For μ -a.e. $(e, \omega_{\partial A})$ we have*

$$\mathcal{E}(e, \omega_{\partial A}) \neq \emptyset \text{ and } \nabla H_A := \left(\frac{\partial H_A}{\partial p_i}, \frac{\partial H_A}{\partial q_i} \right)_{i \in A} \neq 0 \text{ on } \mathcal{E}(e, \omega_{\partial A}).$$

Proof. Applying Sard's theorem to $H_A(\omega_A | \omega_{\partial A})$ as a function of $\omega_A \in (\mathbb{R} \times \mathbb{R})^A$ with fixed $\omega_{\partial A}$ (see e.g. [St]), we see that the statement

$$\mathcal{E}(e, \omega_{\partial A}) = \emptyset \text{ or } \nabla H_A \neq 0 \text{ on } \mathcal{E}(e, \omega_{\partial A})$$

holds for almost every $e \in \mathbb{R}$ and for every $\omega_{\partial A}$. Especially, we see that the relation above holds for a.e. $(e, \omega_{\partial A}) \in \mathbb{R} \times (\mathbb{R} \times \mathbb{R})^{\partial A}$ with respect to Lebesgue measure, $ded\omega_{\partial A}$. However, since $\mu \in \mathcal{P}_0(\Omega)$, its restriction to $\mathcal{A}_{A \cup \partial A}$ is absolutely continuous with respect to Lebesgue measure $d\omega_{A \cup \partial A}$, thus recalling the concrete form of $H_A(\omega_A | \omega_{\partial A})$, we see that the joint distribution of $e = H_A(\omega_A | \omega_{\partial A})$ and $\omega_{\partial A}$ is absolutely continuous with respect to Lebesgue measure, thus the previous relation holds for μ -a.e. $(e, \omega_{\partial A})$. Since $\mathcal{E}(e, \omega_{\partial A}) \neq \emptyset$ μ -a.e., this completes the proof. $\square$

Remark 4.1 Lemma 4.1 implies by the implicit function theorem that $\mathcal{E}(e, \omega_{\partial A})$ is a compact $(2|A|-1)$ -dimensional manifold for μ -a.e. $(e, \omega_{\partial A})$. $\square$

Lemma 4.2 *For μ -a.e. (e, ω_{A^c}) ,*

$$\int_{\mathcal{E}(e, \omega_{\partial A})} L^i \varphi d\mu_{e, \omega_{A^c}} = 0, \quad \varphi \in C^\infty(\mathcal{E}(e, \omega_{\partial A})), \quad i \in A,$$

where $\mu_{e, \omega_{A^c}}$ denotes the conditional distribution of μ given ω_{A^c} and $H_A = e$.

Proof. This is an easy consequence of (MIP) by noting that

$$L^i \psi = \psi_1 \psi_2 L^i \varphi, \quad i \in A$$

for any smooth $\psi(\omega) = \varphi(\omega_A) \psi_1(H_A(\omega_A | \omega_{\partial A})) \psi_2(\omega_{A^c})$. $\square$

From now on we fix $(e, \omega_{\partial A})$ such that the conclusion of Lemma 4.1 holds true, and denote simply by $\mathcal{E}$ the corresponding energy shell. If X and Y are C^∞ -vector fields over $\mathcal{E}$ then the Lie bracket $[X, Y] = XY - YX$ is defined in the usual way. Let $\mathbf{L}_0$ be the Lie algebra generated by $\{L^i\}_{i \in A}$ with real coefficients, i.e. $\mathbf{L}_0$ is the real vector space spanned by $\{L^I; I \in \bigcup_{n=1}^{\infty} A^n\}$, where

$$L^I = [L^{i_1}, [L^{i_2}, [\dots, [L^{i_{n-1}}, L^{i_n}] \dots]]]$$

for $I = (i_1, i_2, \dots, i_n) \in A^n$. We are going to verify the following Hörmander type condition:

$$\dim \mathbf{L}_0(\omega_A) = 2|A| - 1 \quad \text{for every } \omega_A \in \mathcal{E}, \quad (4.1)$$

where $\mathbf{L}_0(\omega_A) = \{R(\omega_A) \in T_{\omega_A} \mathcal{E}; R \in \mathbf{L}_0\}$ and $T_{\omega_A} \mathcal{E}$ denotes the space of tangent vectors at ω_A .

Proposition 4.1 *If $A \subset \mathbb{Z}^d$ is connected, then the family $\{L^i\}_{i \in A}$ satisfies (4.1).*

Remark 4.2 Let Θ be an open subset of $\mathcal{E}$ and denote $\mathbf{L}(\Theta)$ the Lie algebra generated by $\{L^i\}_{i \in A}$ with coefficients from $C^\infty(\Theta)$; namely

$$\mathbf{L}(\Theta) = \left\{ \sum_{j=1}^n a_j R^j |_{\Theta} \in \mathcal{X}(\Theta); a_j \in C^\infty(\Theta), R^j \in \mathbf{L}_0, n = 1, 2, \dots \right\},$$

where $\mathcal{X}(\Theta)$ is the family of vector fields on Θ . Then (4.1) is equivalent to the following condition: Each $\omega_A \in \mathcal{E}$ has an open neighborhood Θ such that $\dim \mathbf{L}(\omega_A; \Theta) = 2|A| - 1$, where

$$\mathbf{L}(\omega_A; \Theta) = \{R(\omega_A) \in T_{\omega_A} \mathcal{E}; R \in \mathbf{L}(\Theta)\}.$$

In fact, this is shown by means of an identity

$$[fX, gY] = fg[X, Y] + f(Xg)Y - g(Yf)X \quad \text{for } X, Y \in \mathcal{X}(\Theta), f, g \in C^\infty(\Theta);$$

see Lemma 1.1 in [K], page 161. $\square$

Let us introduce the following vector fields on $\mathcal{E}$:

$$X^{jk} := p_k \frac{\partial}{\partial q_j} - H_j \frac{\partial}{\partial p_k}, \quad Y^{jk} := p_k \frac{\partial}{\partial p_j} - p_j \frac{\partial}{\partial p_k}, \quad Z^{jk} := H_k \frac{\partial}{\partial q_j} - H_j \frac{\partial}{\partial q_k},$$

for $i, j, k \in A$; moreover

$$H_i \equiv H_i(\omega_A) := \frac{\partial H_A}{\partial q_i}(\omega_A | \omega_{\partial A}), \quad H_{ij} \equiv H_{ij}(\omega_A) := \frac{\partial^2 H_A}{\partial q_i \partial q_j}(\omega_A | \omega_{\partial A}),$$

and so on. Notice that $L^i = X^{ii}$, $Y^{kj} = -Y^{jk}$ and $Z^{kj} = -Z^{jk}$. Then the proof of the proposition is concluded if we can verify that every $\omega_A \in \mathcal{E}$ has an open neighborhood Θ such that

$$X^{jk}, Y^{jk}, Z^{jk} \in \mathbf{L}(\Theta) \quad \text{for } j, k \in A. \quad (4.2)$$

Indeed, the conclusion of Lemma 4.1 implies that for each $\omega_A \in \mathcal{E}$ there exists an $i \in A$ such that $p_i \neq 0$ or $H_i \neq 0$. Therefore, according as $p_i \neq 0$ or $H_i \neq 0$, the families

$$\{\{X^{ji}\}_{j \in A}, \{Y^{ji}\}_{j \in A \setminus \{i\}}\} \text{ or } \{\{X^{ij}\}_{j \in A}, \{Z^{ij}\}_{j \in A \setminus \{i\}}\}$$

consist of $(2|A| - 1)$ linearly independent tangent vectors at ω_A , respectively, which proves (4.1), see Remark 4.2. Before proving (4.2), we summarize some fundamental commutation relations, they can be verified by simple calculations.

Lemma 4.3

- (1) $[L^i, X^{jk}] = H_{ij} Y^{ik} + \delta_{ik} Z^{ij}$
- (2) $[L^i, Y^{jk}] = -\delta_{ij} X^{ik} + \delta_{ik} X^{ij}$
- (3) $[Y^{jk}, Y^{\ell k}] = Y^{j\ell}$ if j, k, ℓ are different,
- (4) $[Y^{jk}, X^{k\ell}] = 0$ if j, k, ℓ are different.

Remark 4.3 It can be shown that the Lie algebra generated by $\{X^{jk}, Y^{jk}, Z^{jk}\}_{j,k \in A}$ with $C^\infty(\Theta)$ coefficients coincides with the linear space over the module $C^\infty(\Theta)$ spanned by $\{X^{jk}, Y^{jk}, Z^{jk}\}_{j,k \in A}$. $\square$

The following relations are also useful.

Corollary 4.1 If $i \neq k$, then we have

- (5) $H_{ik} Y^{ik} = [L^i, L^k]$
- (6) $X^{ik} = -[L^i, Y^{ik}]$
- (7) $X^{ki} = [L^k, Y^{ik}]$
- (8) $Z^{ik} = [L^i, X^{ki}]$ $\square$

Now we prove (4.2) by induction. We fix $\omega_A \in \mathcal{E}$ and $i \in A$ such that at least one of the relations $p_i \neq 0$ or $H_i \neq 0$ holds true at ω_A . The first step of the argument is:

Lemma 4.4 There exists an open neighborhood Θ of ω_A such that (4.2) holds for all $j, k \in \Gamma$ if $\Gamma = \{i, m\}$ with $m \in A$: $|i - m| = 1$.

Proof. Suppose first that $H_{im} \neq 0$, then (5) implies $Y^{im} \in \mathbf{L}(\Theta)$, therefore

$$X^{im}, X^{mi}, Z^{im} \in \mathbf{L}(\Theta)$$

by (6)–(8); provided that Θ is sufficiently small. Suppose now that $H_{im} = 0$, then $H_{iim} \neq 0$ by assumption, thus from (2) we get

$$[L^i, [L^i, L^m]] = [L^i, H_{im} Y^{im}] = p_i H_{iim} Y^{im} - H_{im} X^{im} \in \mathbf{L}(\Theta), \quad (4.3)$$

while from (2) and (1)

$$\begin{aligned} & [L^i, [L^i, [L^i, L^m]]] \\ &= \{-H_i H_{iim} + p_i^2 H_{iim} - H_{im} H_{ii}\} Y^{im} - 2p_i H_{iim} X^{im} \in \mathbf{L}(\Theta), \end{aligned} \quad (4.4)$$

finally

$$\begin{aligned} & [L^i, [L^i, [L^i, [L^i, L^m]]]] \\ &= \{3H_i H_{iim} - 3p_i^2 H_{iim} + H_{im} H_{ii}\} X^{im} + f(p, q) Y^{im} \in \mathbf{L}(\Theta) \end{aligned} \quad (4.5)$$

with some $f \in C^\infty(\Theta)$. Remember that $p_i \neq 0$ or $H_i \neq 0$ at ω_A . If $p_i \neq 0$ and $H_{im} = 0$, then $p_i H_{im} \neq 0$, thus from (4.3) and (4.4) we obtain that $Y^{im} \in \mathbf{L}(\Theta)$ if Θ is small. On the other hand, if $p_i = 0$ and $H_i \neq 0$, then (4.4) and (4.5) imply $Y^{im} \in \mathbf{L}(\Theta)$ by a similar argument. Therefore, even if $H_{im} = 0$, the conclusion follows from (6)–(8) as before. $\square$

Consider now the set $\Gamma_0 = \{m \in A; |i - m| = 0 \text{ or } 1\}$, we have

Lemma 4.5 (4.2) holds for all $j, k \in \Gamma_0$.

Proof. From the commutation relation (3) and Lemma 4.4 we see that $Y^{jk} \in \mathbf{L}(\Theta)$ for every $j, k \in \Gamma_0$. Therefore, from (6)–(8), $X^{jk}, Z^{jk} \in \mathbf{L}(\Theta)$ for every $j, k \in \Gamma_0$. $\square$

To terminate the procedure of induction, suppose (4.2) for a connected subset $\Gamma \subset A$ containing Γ_0 . Choose $\ell \in A \setminus \Gamma$ and $m \in \Gamma$ such that $|\ell - m| = 1$. We have the following lemma.

Lemma 4.6 There exists a neighborhood Θ of ω_A such that (4.2) holds true for all $j, k \in \Gamma \cup \{\ell\}$.

Proof. Since the case of $H_{m\ell} \neq 0$ can easily be treated as before by noting that $[L^m, L^\ell] = H_{m\ell} Y^{m\ell}$ yields $Y^{m\ell} \in \mathbf{L}(\Theta)$, at least if Θ is sufficiently small, we may assume that $H_{m\ell} = 0$. We have

$$[L^m, [L^m, L^\ell]] = p_m H_{mm\ell} Y^{m\ell} - H_{m\ell} X^{m\ell} \in \mathbf{L}(\Theta). \quad (4.6)$$

However, $H_{m\ell} = 0$ implies $H_{mm\ell} \neq 0$ at ω_A while p_m might vanish. To overcome this inconvenience, we choose a path $\{m = m_0, m_1, m_2, \dots, m_N = i\}$ in Γ such that $|m_p - m_{p+1}| = 1$ for $0 \leq p \leq N-1$ and $m_p \neq m_q$ if $p \neq q$. By induction we show that

$$\begin{aligned} & [Y^{i, m_{N-1}}, [Y^{m_{N-1}, m_{N-2}}, [\dots, [Y^{m_1, m}, p_m Y^{m\ell}] \dots]]] \\ & = (-1)^N p_i Y^{m\ell} + (-1)^N p_m Y^{i\ell}. \end{aligned} \quad (4.7)$$

Since (4) yields $[Y^{m_1, m}, X^{m\ell}] = 0$, we obtain from (4.6) and (4.7) that

$$\begin{aligned} & (-1)^N [Y^{i, m_{N-1}}, [Y^{m_{N-1}, m_{N-2}}, [\dots, [Y^{m_1, m}, [L^m, [L^m, L^\ell]]] \dots]]] \\ & = p_i H_{mm\ell} Y^{m\ell} + p_m H_{mm\ell} Y^{i\ell} \in \mathbf{L}(\Theta). \end{aligned} \quad (4.8)$$

Hence by $H_{mm\ell} \neq 0$ at ω_A we get

$$p_i Y^{m\ell} + p_m Y^{i\ell} \in \mathbf{L}(\Theta) \quad (4.9)$$

at least if Θ is sufficiently small. Furthermore, we have

$$\frac{1}{2} [Y^{im}, p_i Y^{m\ell} + p_m Y^{i\ell}] = p_m Y^{m\ell} - p_i Y^{i\ell} \in \mathbf{L}(\Theta), \quad (4.10)$$

$$[L^i, p_m Y^{m\ell} - p_i Y^{i\ell}] = H_i Y^{i\ell} + p_i X^{i\ell} \in \mathbf{L}(\Theta), \quad (4.11)$$

and

$$\frac{1}{2} [L^i, H_i Y^{i\ell} + p_i X^{i\ell}] = p_i H_{ii} Y^{i\ell} - H_i X^{i\ell} \in \mathbf{L}(\Theta), \quad (4.12)$$

again if Θ is sufficiently small. Now suppose $p_i \neq 0$, then from (4.9) and (4.10)

$$\{p_i^2 + p_m^2\} Y^{m\ell} = p_i \{p_i Y^{m\ell} + p_m Y^{i\ell}\} + p_m \{p_m Y^{m\ell} - p_i Y^{i\ell}\} \in \mathbf{L}(\Theta)$$

so that $Y^{m\ell} \in \mathbf{L}(\Theta)$. On the other hand, if $p_i = 0$ and $H_i \neq 0$, then we have $Y^{i\ell} \in \mathbf{L}(\Theta)$ from (4.11) and (4.12). Therefore by (3) we have in both cases $Y^{j\ell} \in \mathbf{L}(\Theta)$ for every $j \in \Gamma \cup \{\ell\}$, which completes the proof as before. $\square$

In view of (4.2) this completes the proof of Proposition 4.1. $\square$

Now, we are in a position to complete the proof of Theorem 3.3 by means of Proposition 4.1.

Lemma 4.7 Assume that $\Lambda \subset \mathbb{Z}^d$ is finite and connected. Then, for μ -a.e. (e, ω_{Λ^c}) , $\mu_{e, \omega_{\Lambda^c}}$ admits a smooth density $f = f_{e, \omega_{\Lambda^c}} \in C^\infty(\mathcal{E}(e, \omega_{\partial\Lambda}))$ with respect to the surface measure $d\tilde{\omega}_\Lambda$ on $\mathcal{E}(e, \omega_{\partial\Lambda})$, namely $\mu_{e, \omega_{\Lambda^c}}(d\tilde{\omega}_\Lambda) = f(\tilde{\omega}_\Lambda) d\tilde{\omega}_\Lambda$.

Proof. Consider the second order differential operator G on $\mathcal{E} = \mathcal{E}(e, \omega_{\partial\Lambda})$, see (3.12). Then from Lemma 4.2

$$\int_{\mathcal{E}} G\varphi d\mu_{e, \omega_{\Lambda^c}} = 0 \text{ if } \varphi \in C^\infty(\mathcal{E}). \quad (4.13)$$

Since the coefficients of G are smooth, the martingale problem associated with G is well-posed, thus from (4.13) we obtain that $\mu_{e, \omega_{\Lambda^c}}$ is an invariant measure of the diffusion generated by G :

$$\mu_{e, \omega_{\Lambda^c}}(d\tilde{\omega}_\Lambda) = \int_{\mathcal{E}} P(t, \omega_\Lambda, d\tilde{\omega}_\Lambda) \mu_{e, \omega_{\Lambda^c}}(d\omega_\Lambda) \text{ for } t > 0,$$

where $P(t, \omega_\Lambda, d\tilde{\omega}_\Lambda)$ is the transition probability of this diffusion (see [E]). However, from Proposition 4.1 and Hörmander's theorem it follows that $P(t, \omega_\Lambda, d\tilde{\omega}_\Lambda)$ admits a smooth density $p(t, \omega_\Lambda, \tilde{\omega}_\Lambda) \in C^\infty((0, \infty) \times \mathcal{E} \times \mathcal{E})$ with respect to $d\tilde{\omega}_\Lambda$ (see e.g. [IK]). $\square$

The final step of the argument is based on

Lemma 4.8 Assume that Λ is finite and connected. Then the density f introduced in Lemma 4.7 is constant on each connected component of $\mathcal{E} = \mathcal{E}(e, \omega_{\partial\Lambda})$ for μ -a.e. (e, ω_{Λ^c}) .

Proof. We use the result of controllability of nonlinear symmetric systems of ordinary differential equations, which is known as a consequence of Chow's theorem (see [He] or [SJ]). In fact, Hörmander's condition (4.1) implies that the system

$$\frac{dx(t)}{dt} = F(x(t), u(t)) \quad (4.14)$$

with

$$F(\cdot, u) = \sum_{i \in \Lambda} u_i L^i \in \mathcal{X}(\mathcal{E}) \text{ for } u = (u_i)_{i \in \Lambda} \in \mathbb{R}^\Lambda$$

is controllable on each connected component of $\mathcal{E}$. Namely, for every pair $\omega_\Lambda^{(1)}$ and $\omega_\Lambda^{(2)}$ belonging to the same component of $\mathcal{E}$ one can find a piecewise constant function $u = u(t): [0, 1] \rightarrow \mathbb{R}^\Lambda$ (i.e., $u \equiv \text{const}$ on $[t_{i-1}, t_i]$, $1 \leq i \leq n-1$, and on $[t_{n-1}, t_n]$ for some finite partition $0 = t_0 < t_1 < \dots < t_n = 1$ of $[0, 1]$) such that the

corresponding solution of (4.14) connects $\omega_A^{(1)}$ and $\omega_A^{(2)}$ in the sense that $x(0) = \omega_A^{(1)}$ and $x(1) = \omega_A^{(2)}$. Since by Lemma 4.2 $(L^i)^* f = 0$ on $\mathcal{E}$, we have

$$\frac{d}{dt} f(x(t)) = \sum_{i \in A} u_i(t) (L^i f)(x(t)) = 0, \quad \text{for } t \neq t_i, i = 1, 2, \dots, n-1$$

along the controlled solution $x(t)$ of (4.14), consequently $f(\omega_A^{(1)}) = f(\omega_A^{(2)})$. Indeed, we have $(L^i)^* = -L^i$ with respect to $d\omega_{A \cup \partial A}$ on $(\mathbb{R} \times \mathbb{R})^{A \cup \partial A}$ thus it holds true on each energy shell $\mathcal{E}$ with respect to $d\tilde{\omega}_A$. $\square$

Theorem 3.3 has only been proven for connected $A \subset \mathbb{Z}^d$, whence the general statement follows immediately.

5 Construction of random evolutions

The evolution with random velocity reflections, i.e. with $\mathcal{G}_{\text{ran}} = \mathcal{G}^R$, can be defined as follows. For each site $k \in \mathbb{Z}^d$ we have independent Poisson processes N_k of intensity $a > 0$, where $N_k(t)$ is the number of points in the interval $(0, t]$. Let $\mathcal{X}_k(t) = (-1)^{N_k(t)}$, then for almost every realization of the random element $N^R = (N_k)_{k \in \mathbb{Z}^d}$ we have a set of integral equations:

$$\begin{aligned} p_k(t) &= \mathcal{X}_k(t) \left(p_k(0) - \int_0^t \mathcal{X}_k(s) \frac{\partial H(\omega(s))}{\partial q_k} ds \right), \\ q_k(t) &= q_k(0) + \int_0^t p_k(s) ds \quad \text{for } k \in \mathbb{Z}^d. \end{aligned} \quad (5.1)$$

The case of velocity exchanges is similar, but a little bit more complicated. Here we have independent Poisson processes indexed by the bonds of $\mathbb{Z}^d$, i.e. $N_{k,j} = N_{j,k}$ for $|j-k|=1$, where $N_{k,j}(t)$ denotes the number of points in $(0, t]$; the intensity of each process is again $a > 0$. The following system is well defined for almost every realization of $N^E = (N_{k,j})_{|j-k|=1}$.

$$\begin{aligned} p_k(t) &= \sum_{j \in \mathbb{Z}^d} \left(\delta_{k,j}(t, 0) p_j(0) - \int_0^t \delta_{k,j}(t, s) \frac{\partial H(\omega(s))}{\partial q_j} ds \right), \\ q_k(t) &= q_k(0) + \int_0^t p_k(s) ds \quad \text{for } k \in \mathbb{Z}^d, \end{aligned} \quad (5.2)$$

where δ is the fundamental solution to the trivial problem of $U \equiv V \equiv 0$, i.e. then $p_k(t) = \sum_{j \in \mathbb{Z}^d} \delta_{k,j}(t, s) p_j(s)$ for $0 \leq s \leq t < +\infty$ and $k, j \in \mathbb{Z}^d$. More exactly, δ is the permutation kernel of the stirring process induced by N^E as follows. Let $\xi_i(s)$ denote the walk started from $i \in \mathbb{Z}^d$ at time 0 and jumping to the opposite end of the bond on which the next point appears. This system of random walks is uniquely determined by the requirements that $\xi_i(t)$ is a right continuous function of $t \geq 0$ such that $\xi_i(t) = k$ at $t > s$ if $\xi_i(s) = j$ and $N_{j,k}(t) = N_{j,k}(s) + 1$ but $N_{j,l}(t) = N_{j,l}(s)$ for $l \neq k$ and $|l-j|=1$, while $\xi_i(t) = \xi_i(s)$ at $t > s$ if $\xi_i(s) = j$ and $N_{j,k}(t) = N_{j,k}(s)$ for all $k \in \mathbb{Z}^d$ with $|k-j|=1$. Let $\eta_i(j, s) = 1$ if $\xi_i(s) = j$ and $\eta_i(j, s) = 0$ otherwise, then

$$\delta_{k,j}(t, s) = \sum_{i \in \mathbb{Z}^d} \eta_i(k, t) \eta_i(j, s) \quad N^E\text{-a.s.}$$

Both (5.1) and (5.2) can be solved in Ω for almost every realization of N^R and N^E , respectively, and the solution is a continuous and differentiable function of initial data. The basic tool of the derivation is the following system of integral inequalities for $u_k \geq 0$, $k \in \mathbb{Z}^d$, where $v_k \geq 0$ and $\gamma_{k,j} \geq 0$ are given functions, and K is a constant depending only on U and V :

$$u_k(t) \leq v_k(t) + K \sum_{j \in \mathbb{Z}^d} \int_0^t \gamma_{k,j}(t, s) u_j(s) ds. \quad (5.3)$$

For example, if $u_k(t) = |p_k(t)|$, then in the first case we have $\gamma_{k,j}(t, s) = K(t-s)$ if $|j-k| \leq 1$, and $\gamma_{k,j} = 0$ otherwise, while

$$v_k(t) = |p_k(0)| + \sum_{|j-k| \leq 1} (K + |q_j(0)|)t.$$

In the case of (5.2) we have again (5.3) for $u_k(t) = |p_k(t)|$ with the same constant K and

$$\begin{aligned} \gamma_{k,j}(t, s) &= \sum_{|i-j| \leq 1} \int_s^t \delta_{k,i}(t, \tau) d\tau \\ v_k(t) &= \sum_{j \in \mathbb{Z}^d} (\delta_{k,j}(t, 0) |p_j(0)| + \gamma_{k,j}(t, 0) (K + |q_j(0)|)). \end{aligned}$$

Let us remark that the mean value of $\delta_{k,j}(t, s)$ is just the transition probability of a symmetric simple random walk with jump rate a , thus it is easy to get bounds on the integral operator with kernel γ also in this case.

The system above can be solved by a direct iteration procedure, we get

$$u_k(t) \leq v_k(t) + \sum_{m=1}^{\infty} K^m \sum_{j \in \mathbb{Z}^d} \int_0^t \gamma_{k,j}^{(m)}(t, s) v_j(s) ds, \quad (5.4)$$

where $\gamma^{(1)} = \gamma$, and

$$\gamma_{k,j}^{(m+1)}(t, s) = \sum_{i \in \mathbb{Z}^d} \int_s^t \gamma_{k,i}^{(m)}(t, \tau) \gamma_{i,j}(\tau, s) d\tau. \quad (5.5)$$

Let $\mathbf{X}$ denote the space of real sequences $x = (x_k)_{k \in \mathbb{Z}^d}$, a strong topology of $\mathbf{X}$ is defined by means of a family of Hilbert norms, $|\cdot|_\alpha$ given for $\alpha > 0$ by

$$|x|_\alpha^2 = \sum_{k \in \mathbb{Z}^d} \exp(-\alpha|k|) |x_k|^2, \quad (5.6)$$

thus $\|\omega\|_\alpha = |x|_\alpha$ with $x_k = (p_k^2 + q_k^2)^{1/2}$ if $\omega = (p_k, q_k)_{k \in \mathbb{Z}^d}$. The convergence of a sequence in the strong topology of Ω means convergence with respect to every norm $\|\cdot\|_\alpha$, $\alpha > 0$; the space of strongly continuous $\varphi: \Omega \rightarrow \mathbb{R}$ will be denoted by $C_s(\Omega)$. The reason why we have introduced a whole family of norms instead of a single one is quite simple. The strongly bounded sets of $\mathbf{X}$ or those of Ω are weakly compact, and the relative weak topology coincides with the strong one on each strongly bounded set, thus moment conditions allow us to avoid a sharp distinction of weak and strong compactness. Now we show that the kernels γ are contractive in the following sense.

Lemma 5.1 *For each $T > 0$ there exists a positive number $\alpha(T)$, and for $0 < \alpha < \alpha(T)$ we have also a random variable $C(\alpha, T)$ such that if $v_k(t) \leq \tilde{v}_k$ for all $t \leq T$ and $k \in \mathbb{Z}^d$,*

then (5.4) and (5.5) imply

$$|u(t)|_\alpha \leq C(T) |\tilde{v}|_\alpha \quad \text{for each } 0 \leq t \leq T.$$

$C(\alpha, T)$ depends only on K and d in the case of (5.1); it does depend on the random element N^E in the second case, but its second moment is finite.

Proof. The first case is trivial, we can calculate each term of expansion (5.6), and we obtain a deterministic bound for every $\alpha > 0$. In the second case we can use the reflection principle to determine the distribution of $\zeta_{k,j}(s, T)$,

$$\zeta_{k,j}(s, T) = \sup_{s < t < T} \delta_{k,j}(t, s) \quad \text{for } 0 < s < T.$$

In this way we obtain a bound

$$\mathbf{E}^E \left(\sup_{0 < s < t < T} \gamma_{k,j}(t, s) \right) \leq \exp[-\alpha(T)|k-j|],$$

where $\mathbf{E}^E$ denotes the expectation with respect to the random element N^E . Observe now that the factors γ of the terms of the expansion on the right hand side of (5.6) are independent, thus the proof is completed by the elementary fact

$$\sup_{j \in \mathbb{Z}^d} \sum_{k \in \mathbb{Z}^d} \exp[-\alpha|k| + \alpha|j| - \beta|k-j|] < +\infty \quad \text{if } 0 < \alpha < \beta.$$

Indeed, as $\delta_{k,j}$ is either 0 or 1, we can use the Schwarz inequality with weights 2^{-m} for the sum, and with uniform weights for the multiple integrals to derive the conclusion from the above estimates by a direct calculation. $\square$

This simple tool is sufficient to construct regular solutions in Ω .

Theorem 5.1 *If U'' and V'' are bounded, then both (5.1) and (5.2) admit uniquely defined solutions $\omega_t = \mathcal{U}_R^t \omega$ and $\omega_t = \mathcal{U}_E^t \omega$ for every initial configuration $\omega_0 = \omega \in \Omega$, and for almost every random element $N = N^R$ or $N = N^E$, respectively. The solutions remain in Ω , and they are strongly continuous functions of initial data.*

Proof. In view of Lemma 5.1 this argument is quite standard, so we sketch only the main steps. We start with a sequence of partial dynamics allowing only a finite number of coordinates to vary. Choosing u_k and v_k as specified after (5.3) we show via Lemma 5.1 that the velocities are bounded on compact intervals of time. Therefore, by the Arzela-Ascoli Theorem we have limiting solutions for every initial configuration, and for almost every realization of the random elements N^R and N^E , respectively. To conclude the uniqueness of solutions, as well as their continuous dependence on initial data, we define $u_k(t)$ as the magnitude of the difference of the velocities of two solutions, and use again Lemma 5.1. $\square$

The Markov semigroups of our random evolutions are defined by

$$\mathcal{P}_R^t \varphi(\omega) = \mathbf{E}^R \varphi(\mathcal{U}_R^t \omega) \quad \text{and} \quad \mathcal{P}_E^t \varphi(\omega) = \mathbf{E}^E \varphi(\mathcal{U}_E^t \omega) \quad \text{for } \varphi \in C_s(\Omega), \quad (5.7)$$

respectively, where $\mathbf{E}^R$ and $\mathbf{E}^E$ denote expectations with respect to the random elements N^R and N^E . It is easy to check that they are really generated by $\mathcal{L} + a\mathcal{G}^R$ and by $\mathcal{L} + a\mathcal{G}^E$, respectively. In view of Theorem 5.1, both semigroups map $C_s(\Omega)$ into itself. If the initial configuration is distributed by $\mu \in \mathcal{P}(\Omega)$, then $\mu_t = \mu \mathcal{P}_R^t$ and $\mu_t = \mu \mathcal{P}_E^t$ denote the evolved states of the corresponding random dynamics. Since the dynamics preserve moment conditions, Theorem 2.3 is obtained as a direct

consequence of Theorem 5.1. Moreover, under the condition $\bar{I}[\mu_0] \leq K$ with $K < \infty$ being fixed, the evolved state depends in a weakly continuous way on the initial distribution μ_0 , see the entropy bounds of the next section.

The following form of differentiable dependence on initial data shall play an important role in estimating the boundary terms of entropy production, see (6.2)–(6.5), it is based on Donsker–Varadhan type rate functions of the following art.

Definition 5.1 Suppose that Γ is the generator of a Markov process in Ω and $\mathcal{B} \subset \mathcal{A}$ is a σ -field such that the domain of Γ consists of $\mathcal{B}$ -measurable functions, and Γ maps its domain, $\text{Dom } \Gamma$ into $\mathcal{B}$ -measurable functions. Then the rate of $\mu \in \mathcal{P}(\Omega)$ with respect to Γ and $\mathcal{B}$ is defined as

$$D_{\mathcal{B}}^{\Gamma}[\mu] = 4 \sup_{\delta > 0} \sup_{\psi \in \text{Dom } \Gamma} \left\{ \int -\frac{\Gamma\psi}{\psi} d\mu : \psi > \delta \text{ and } -\Gamma\psi < \frac{1}{\delta} \right\}.$$

If $\mathcal{B} = \mathcal{A}_n$ and $\Gamma = \mathcal{G}_{k,1}^P$, for $k \in A_n$ or $\Gamma = \mathcal{G}_{k,1}^Q$ for $k \in A_{n-1}$, then the abbreviations $D_{n,k}^P[\mu]$ and $D_{n,k}^Q[\mu]$ are used, cf. (3.1). If $\mathcal{B} = \mathcal{A}$ then the subscript n is omitted.

Let us remark that the volume terms of entropy production D_n^E and D_n^R are not rate functions of this kind. For a comprehensive study of rate functions see [DV] or [DS]. Monotonicity with respect to $\mathcal{B}$, and convexity and lower semi-continuity in μ are the most useful properties of D^{Γ} .

In particular, for $k \in \mathbb{Z}^d$,

$$\bar{D}_k^P[\mu] \equiv D_k^P[\mu] = \sup_{n \geq 0} D_{n,k}^P[\mu] \quad \text{and} \quad \bar{D}_k^Q[\mu] \equiv D_k^Q[\mu] = \sup_{n \geq 1} D_{n,k}^Q[\mu], \quad (5.8)$$

and if $\mu \in \mathcal{P}(\Omega)$ is translation invariant, then

$$\begin{aligned} \bar{D}^P[\mu] &:= \bar{D}_k^P[\mu] = \sup_{n \geq 0} (2n+1)^{-d} \sum_{k \in A_n} D_{n,k}^P[\mu], \\ \bar{D}^Q[\mu] &:= \bar{D}_k^Q[\mu] = \sup_{n \geq 1} (2n-1)^{-d} \sum_{k \in A_{n-1}} D_{n,k}^Q[\mu]. \end{aligned} \quad (5.9)$$

Suppose now that $d\mu = f_n d\lambda_n^0$ on $\mathcal{A}_n$ and $f_n \in C_0^2(\Omega)$ is bounded away from zero, then using (KMSP) or (KMSQ), we can replace the integrands in the definitions of D^P or D^Q by expressions like

$$\left(\frac{f_n}{\psi} \right)' \psi' = \left(\frac{f_n'}{f_n} \frac{\psi'}{\psi} - \left(\frac{\psi'}{\psi} \right)^2 \right) f_n \leq \frac{1}{4} \left(\frac{f_n'}{f_n} \right)^2 f_n, \quad (5.10)$$

where prime denotes the corresponding derivative. This means that the supremum is attained for $\psi = \sqrt{f_n}$, consequently

$$\begin{aligned} D_{n,k}^P[\mu] &= \int \left(\frac{1}{f_n} \frac{\partial f_n}{\partial p_k} \right)^2 d\mu \quad \text{for } k \in A_n, \\ D_{n,k}^Q[\mu] &= \int \left(\frac{1}{f_n} \frac{\partial f_n}{\partial q_k} \right)^2 d\mu \quad \text{for } k \in A_{n-1}. \end{aligned} \quad (5.11)$$

It is less obvious, that the finiteness of D^{Γ} implies the existence and the necessary smoothness of f_n (see [DV], [DS]).

If the evolution does not create smoothness of local densities then the control of terms like D^P and D^Q should be based on differentiable dependence of solutions on initial data.

Observe that $u_k(t) = |\partial p_k(t)/\partial p_j(0)|$ and $u_k(t) = |\partial p_k(t)/\partial q_j(0)|$ also satisfy (5.3) with suitably chosen v_k 's, thus Lemma 5.1 yields bounds for the derivatives of the evolved configuration with respect to its initial values. By means of this simple fact we prove:

Lemma 5.2 Suppose that $\bar{D}_k^P[\mu] + \bar{D}_k^Q[\mu] \leq M$ for each $k \in \mathbb{Z}^d$, then we have an increasing function $D(t)$, $t > 0$ such that $D_k^P[\mu \mathcal{P}^t] \leq MD(t)$ both for $\mathcal{P}^t = \mathcal{P}_R^t$ as well as for $\mathcal{P}^t = \mathcal{P}_E^t$.

Proof. First we consider a finite system restricted to Λ_n . This means that we replace H by $H_{\Lambda_n}^0$ both in (5.1) and (5.2), set $N_k(t) \equiv 0$ in (5.1) if $k \notin \Lambda_n$, while $N_{k,j} \equiv 0$ in (5.2) if the bond $\{k, j\}$ is not contained in Λ_n . The evolved configurations will be denoted by $\mathcal{U}_{R,n}^t \omega$ and $\mathcal{U}_{E,n}^t \omega$, respectively, and the initial distribution is μ_n , such that $d\mu_n = f_n d\lambda_n^0$, where f_n is a strictly positive and smooth $\mathcal{A}_n$ -measurable density. Both evolutions preserve λ_n^0 for each realization N of our Poisson processes, thus the density $f_{t,n}^N$ of $\mathcal{U}_{R,n}^t \omega$ or $\mathcal{U}_{E,n}^t \omega$ satisfies $f_{t,n}^N(\omega) = f_n(\mathcal{U}_{R,n}^{-t} \omega)$ or $f_{t,n}^N(\omega) = f_n(\mathcal{U}_{E,n}^{-t} \omega)$, respectively, whence

$$\frac{\partial \sqrt{f_{t,n}^N}}{\partial p_k(t)} = \sum_{j \in \mathbb{Z}^d} \left(\frac{\partial \sqrt{f_n}}{\partial p_j(0)} \frac{\partial p_j(0)}{\partial p_k(t)} + \frac{\partial \sqrt{f_n}}{\partial q_j(0)} \frac{\partial q_j(0)}{\partial p_k(t)} \right).$$

Now we use the Schwarz inequality and the convexity of entropy production to estimate $\bar{D}_k^P[\mu \mathcal{P}^t]$. Since the reversed random trajectories behave in the same way as the original solutions, we can use Lemma 5.1 to handle the right hand side. The situation is even simpler than it was in the proof of Theorem 5.1 because here we need L^∞ bounds, and $\delta_{k,j}$ is a permutation matrix, thus randomness due to $N = N^E$ plays no role at all. The general case follows then by lower semi-continuity of entropy production. $\square$

6 Boundary terms of entropy production

A formal derivation of (ES) and (RS) for the associated random evolutions is almost immediate, but a priori we do not know that any translation invariant stationary state admits smooth local densities; the entropy condition $\bar{I}[\mu] < \infty$ plays a crucial role here. Suppose first that $\mu \in \mathcal{P}(\Omega)$ satisfies $\bar{I}[\mu] < +\infty$ and

$$\bar{D}_k^P[\mu] + \bar{D}_k^Q[\mu] \leq M < +\infty \quad \text{for all } k \in \mathbb{Z}^d, \quad (6.1)$$

then the evolved measure, $\mu_t \in \mathcal{P}(\Omega)$ admits smooth local densities, $f_n = f_n(t, \omega)$ with respect to our reference measures λ_n^0 . The rate of change of I_n consists of the following terms. Since λ_n^0 satisfies (MIC) for $k \in \Lambda_n$ with $H_{\Lambda_n}^0$ instead of H , an easy calculation shows that the Liouville flow yields only a boundary term:

$$\begin{aligned} \int \mathcal{L} \log f_n(t, \omega) \mu_t(d\omega) &= \sum_{k \in \Lambda_n} \int \left(p_k \frac{\partial f_n}{\partial q_k} - \frac{\partial H}{\partial q_k} \frac{\partial f_n}{\partial p_k} \right) \frac{1}{f_n} d\mu_t \\ &= \sum_{k \in \Lambda_n \setminus \Lambda_{n-1}} \int \frac{1}{f_n} \frac{\partial f_n}{\partial p_k} J_{n,k} d\mu_t := B_n^L[\mu_t]; \quad (6.2) \\ J_{n,k}(\omega) &:= \frac{\partial H_{\Lambda_n}^0(\omega)}{\partial q_k} - \frac{\partial H(\omega)}{\partial q_k}. \end{aligned}$$

Note that $J_{n,k}=0$ if $k \in A_{n-1}$. The contribution of random effects is the following, cf. (2.11) and (2.12),

$$\int \mathcal{G}^R \log f_n d\mu_t = -D_n^R[\mu_t], \quad (6.3)$$

$$\int \mathcal{G}^E \log f_n d\mu_t = -D_n^E[\mu_t] + B_n^E[\mu_t]; \quad (6.4)$$

$$B_n^E[\mu_t] := \sum_{k \in A_n} \sum_{\substack{j \notin A_n \\ |j-k|=1}} \int \log \frac{f_n(t, \omega^{k,j})}{f_n(t, \omega)} \mu(d\omega).$$

Comparing the calculations above we get

$$I_n[\mu_t] + a \int_0^t D_n[\mu_s] ds \leq I_n[\mu_0] + \int_0^t B_n[\mu_s] ds, \quad (6.5)$$

where $D_n = D_n^R$, $B_n = B_n^L$ if $\mathcal{G}_{ran} = \mathcal{G}^R$, see (2.12), (6.2) and (6.3), while $D_n = D_n^E$, $B_n = B_n^L + aB_n^E$ if $\mathcal{G}_{ran} = \mathcal{G}^E$, see (2.11), (6.2) and (6.4).

The boundary terms of entropy production can be estimated as follows. From Lemma 5.2 by the Schwarz inequality we get

$$B_n^L[\mu] \leq MD(t)(z_{n+1}^L(t) - z_n^L(t) + |A_n \setminus A_{n-1}|); \quad (6.6)$$

$$\begin{aligned} z_{n+1}^L(t) &:= \sum_{m=1}^n \sum_{k \in A_m \setminus A_{m-1}} \int J_{m,k}(\omega)^2 \mu_t(d\omega) \\ &\leq K_1^\circ(I_{n+1}[\mu_t] + K_2^\circ(1+2n)^d), \end{aligned} \quad (6.7)$$

where the second inequality follows immediately by the variational characterization of entropy (see (2.8) and Definition 2.4).

The second boundary term B_n^E can be treated in the following way. Let $\lambda_{n \vee j}^0$ be a joint distribution of ω_{A_n} and p_j for $j \notin A_n$ such that $d\lambda_{n \vee j}^0 = g(p_j) d\lambda_n^0 dp_j$, where g is the standard normal density, and let $f_{n \vee j}$ denote the corresponding local density of μ_t . Since the velocities are independent with respect to λ_n^0 , we can use the related subadditivity and monotonicity of entropy to conclude that

$$\begin{aligned} B_n^E[\mu_s] &= \sum_{k \in A_n} \sum_{\substack{j \notin A_n \\ |j-k|=1}} \int f_{n \vee j}(s, \omega) \log \frac{f_n(s, \omega^{k,j})}{f_{n \vee j}(s, \omega)} \lambda_{n \vee j}^0(d\omega) \\ &\quad + \sum_{k \in A_n} \sum_{\substack{j \notin A_n \\ |j-k|=1}} \int f_{n \vee j}(s, \omega) \log \frac{f_{n \vee j}(s, \omega)}{f_n(s, \omega)} \lambda_{n \vee j}^0(d\omega) \\ &\leq I_{n+1}[\mu_s] - I_n[\mu_s] + F_n^0 - F_{n+1}^0. \end{aligned} \quad (6.8)$$

At the last step we have exploited also that $H_{A_n}^0 \leq H_{A_{n+1}}^0$. Therefore in both cases we have constants depending on a , T , U and V such that

$$\begin{aligned} B_n[\mu_t] &\leq z_{n+1}(t) - z_n(t), \text{ where} \\ 0 \leq z_n(t) \leq z_{n+1}(t) &\leq K_1(I_{n+1}[\mu_t] + K_2(2n+1)^d) \text{ for } 0 \leq t \leq T. \end{aligned} \quad (6.9)$$

We are facing with a situation described in Lemma 6.1.

Lemma 6.1 Let u_n, v_n and z_n be non-decreasing sequences of non-negative functions of $t \in [0, T]$ such that $z_n = z_n(t) \leq K_1(u_n(t) + K_2(2n-1)^d)$ and

$$u_n(t) + \int_0^t v_n(s) ds \leq u_n(0) + \int_0^t (z_{n+1}(s) - z_n(s)) ds,$$

then for all $n \geq 0$ and $r \in (0, 1)$ we have

$$\begin{aligned} & u_n(t) + \int_0^t v_n(s) ds \\ & \leq \sum_{m=0}^{+\infty} (1-r) r^m ((1+2n+2m)^d K_1 K_2 (1-r)t + \exp[(1-r)K_1 t] u_{n+m}(0)), \end{aligned}$$

whence

$$\limsup_{n \rightarrow \infty} (1+2n)^{-d} \left(u_n(t) + \int_0^t v_n(s) ds \right) \leq \limsup_{n \rightarrow \infty} (1+2n)^{-d} u_n(0) \text{ for } t \leq T.$$

Proof. Using the method of generating functions, by a direct calculation we obtain that

$$\begin{aligned} & \sum_{m=0}^{+\infty} r^m \left(u_{n+m}(t) + \int_0^t v_{n+m}(s) ds \right) \leq \sum_{m=0}^{+\infty} r^m u_{n+m}(0) \\ & + K_1(1-r) \sum_{m=0}^{+\infty} r^m \left(K_2(1+2n+2m)^d t + \int_0^t u_{n+m}(s) ds \right), \end{aligned}$$

whence as u_n and v_n are non-decreasing sequences, by the Grönwall Inequality we get

$$\begin{aligned} & \frac{1}{(1-r)} \left(u_n(t) + \int_0^t v_n(s) ds \right) \leq \sum_{m=0}^{+\infty} r^m \left(u_{n+m}(t) + \int_0^t v_{n+m}(s) ds \right) \\ & \leq K_1 K_2 (1-r)t \sum_{m=0}^{+\infty} r^m (1+2n+2m)^d \\ & + \exp[(1-r)K_1 t] \sum_{m=0}^{+\infty} r^m u_{n+m}(0), \end{aligned}$$

which proves the first statement. Let $\bar{u} := \limsup_{n \rightarrow \infty} (1+2n)^{-d} u_n(0)$, then for any $\varepsilon > 0$ we have an $n_\varepsilon \in \mathbb{N}$ such that for $n > n_\varepsilon$

$$\begin{aligned} & \frac{1}{(1-r)} (1+2n)^{-d} \left(u_n(t) + \int_0^t v_n(s) ds \right) \\ & \leq \sum_{m=0}^{+\infty} r^m \left(\frac{1+2n+2m}{1+2n} \right)^d (K_1 K_2 (1-r)t + \exp[(1-r)K_1 t] (\bar{u} + \varepsilon)). \end{aligned}$$

Now we can send first $n \rightarrow +\infty$, then $r \rightarrow 1$, finally $\varepsilon \rightarrow 0$, which completes the proof of Lemma 6.1. $\square$

Now we are in a position to prove

Proposition 6.1 *If $\mu \in \mathcal{P}_0(\Omega)$ is a stationary state of the evolution $\mathcal{P}_R^1$ or $\mathcal{P}_E^1$, then we have (RS) or (ES), respectively.*

Proof. We have to show that $D_m^R[\mu] = 0$ or $D_m^E[\mu] = 0$, respectively, for each m . Our starting point is the integrated version (6.5) of (2.10). Since our stationary measure, μ need not be as smooth as desired for (6.6), we have to mollify it in such a way that we have (6.1) and $\bar{I}[\mu^\delta] \leq \bar{I}[\mu]$ for its mollified version $\mu^\delta \rightarrow \mu$ as $\delta \rightarrow 0$. The easiest way is to use a reversible evolution as follows.

Let w_k and $\bar{w}_k$ denote independent Wiener processes for $k \in \mathbb{Z}^d$, and consider the following stochastic gradient system:

$$\begin{aligned} dp_k &= -\sigma_k p_k dt + \sqrt{2\sigma_k} dw_k, \\ dq_k &= -\sigma_k \frac{\partial H}{\partial q_k} dt + \sqrt{2\sigma_k} d\bar{w}_k \text{ for } k \in \mathbb{Z}^d, \end{aligned} \quad (6.10)$$

where $\sigma = (\sigma_k)_{k \in \mathbb{Z}^d}$ is a bounded set of non-negative constants. For the construction and regularity properties of such stochastic gradient systems see e.g. [SS]. Let μ_t^σ and f_n^σ denote the state and its local λ_n^0 -densities at time $t > 0$ with initial value $\mu_0^\sigma = \mu$. First we assume that $\sigma_k > 0$ only for a finite number of sites, then we need not worry about smoothness of f_n . We have a uniformly elliptic diffusion, and using (KMSQ), an easy calculation [Fr4] results in

$$\begin{aligned} & \partial_t I_n[\mu_t^\sigma] + \sum_{k \in A_n} \sigma_k D_{n,k}^P[\mu_t^\sigma] + \sum_{k \in A_{n-1}} \sigma_k D_{n,k}^Q[\mu_t^\sigma] \\ &= \sum_{k \in A_n \setminus A_{n-1}} \sigma_k \int \frac{1}{f_n^\sigma} \frac{\partial f_n^\sigma}{\partial q_k} \left(J_{n,k} - \frac{1}{f_n^\sigma} \frac{\partial f_n^\sigma}{\partial q_k} \right) d\mu_t^\sigma \\ &\leq \sum_{k \in A_n \setminus A_{n-1}} \int \frac{\sigma_k}{4} J_{n,k} J_{n,k}^2 d\mu_t^\sigma \leq \frac{\delta}{4} \left(z_{n+1}^L(t) - z_n^L(t) \right), \end{aligned} \quad (6.11)$$

see (6.6) for the definition of z_n , where $\delta > 0$ is a common upper bound of the numbers σ_k .

From the first statement of Lemma 6.1 we obtain an explicit bound for entropy production, see (5.11),

$$\begin{aligned} & \int_0^1 (D_n^{P,\sigma}[\mu_s^\sigma] + D_n^{Q,\sigma}[\mu_s^\sigma]) ds, \text{ where} \\ D_n^{P,\sigma}[\mu] &:= \sum_{k \in A_n} \sigma_k D_{n,k}^P[\mu], \quad D_n^{Q,\sigma}[\mu] := \sum_{k \in A_{n-1}} \sigma_k D_{n,k}^Q[\mu]. \end{aligned}$$

Letting each σ_k go to their least upper bound, say $\delta > 0$, this way we obtain a translation invariant measure μ_t^δ for each $t \geq 0$ with initial value $\mu_0^\delta = \mu$. Set

$$\bar{\mu}^\delta := \int_0^1 \mu_t^\delta dt, \quad (6.12)$$

and remember that $\bar{\mu}^\delta$ converges weakly to our stationary state μ as $\delta \rightarrow 0$. From Lemma 6.1 by convexity and lower semi-continuity of rate functions, cf. (5.8) and (5.9), we get

$$\bar{I}[\bar{\mu}^\delta] + \delta D^P[\bar{\mu}^\delta] + \delta D^Q[\bar{\mu}^\delta] \leq \bar{I}[\mu], \quad (6.13)$$

thus we can apply Lemma 5.2 and Lemma 6.1 to the original, randomized evolutions with initial distribution $\bar{\mu}^\delta$. Let $\tilde{\mu}_t^\delta$ denote the evolved state, we see immediately that (6.5) results in

$$I_n[\tilde{\mu}_t^\delta] + a \int_0^t D_n[\tilde{\mu}_s^\delta] ds \leq I_n[\bar{\mu}^\delta] + \int_0^t (z_{n+1}(s) - z_n(s)) ds,$$

where

$$z_n(t) \leq K_1(I_n[\mu_t] + K_2(1 + 2n)^d) \quad (6.14)$$

with some universal constants K_1 and K_2 . The evolved measure $\tilde{\mu}_t^\delta$ is also translation invariant, therefore for any fixed $m > 0$ by Lemma 6.1 we get

$$\bar{I}[\tilde{\mu}_t^\delta] + a(1 + 2m)^{-d} \int_0^t D_m[\tilde{\mu}_s^\delta] ds \leq \bar{I}[\bar{\mu}^\delta] \leq \bar{I}[\mu], \quad (6.15)$$

which completes the proof by letting δ go to zero. $\square$

Finally, Theorem 2.4 and Theorem 2.5 follow directly from Theorem 2.1, Theorem 3.3 and its Corollary 3.1 by Proposition 6.1.

Remark 6.1 *The existence of translation invariant stationary states also follows by an entropy argument. Starting the process with a smooth $\mu \in \mathcal{P}_0(\Omega)$ we see that the specific entropy $\bar{I}[\bar{\mu}_t]$ of the time averaged distribution $\bar{\mu}_t := t^{-1} \int_0^t \mu_s ds$ remains bounded as $t \rightarrow \infty$. Suppose e.g. that*

$$\lim_{|x| \rightarrow \infty} \frac{U(x)^\delta}{\log(1 + |x|)} = +\infty \text{ for all } \delta > 0,$$

then the family $\bar{\mu}_t$, $t > 0$ is tight with respect to the product topology, and any limit distribution $\bar{\mu}$ is concentrated on Ω . Since $\bar{\mu}$ is a stationary state of finite specific entropy, in this way it is possible to prove the existence of Gibbs states and a statement on the equivalence of ensembles, too.

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