

EXPONENTIAL RELAXATION OF THE NOSÉ-HOOVER THERMOSTAT UNDER BROWNIAN HEATING*

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Abstract. We study a stochastic perturbation of the Nosé-Hoover equation (called the Nosé-Hoover equation under Brownian heating) and show that the dynamics converges at a geometric rate to the augmented Gibbs measure in a weighted total variation distance. The joint marginal distribution of the position and momentum of the particles in turn converges exponentially fast in a similar sense to the canonical Boltzmann-Gibbs distribution. The result applies to a general number of particles interacting through a wide class of potential functions, including the usual polynomial type as well as the singular Lennard-Jones variety.

Keywords. Langevin dynamics; Nosé-Hoover equation; Lennard-Jones potential; geometric ergodicity; molecular dynamics simulation; random sampling.

AMS subject classifications. 60H10; 37A25; 82C31; 60J22; 65C05.

1. Introduction

Efficient sampling from the canonical Boltzmann-Gibbs distribution is a fundamental challenge in molecular dynamics simulation. The most well-known method used to address this challenge is Markov chain Monte Carlo (MCMC) due to Metropolis, Rosenbluth and Rosenbluth [31]. The method is based on random walk proposals to generate unbiased samples from a distribution whose density is known up to a normalization constant. However, it can lead to high correlation. Moreover, even if one corrects for high correlation via the Metropolis step in Hybrid Monte Carlo (HMC) [9, 21], the correction can be computationally expensive in high dimensions due to gradient evaluations.

The method of stochastic gradients has been successful in addressing the cost of such evaluations [1, 3, 34, 44]. The approach is often based on the design of a stochastic differential equation (SDE) whose stationary distribution (or marginal stationary distribution) is the prescribed canonical measure, e.g. Langevin dynamics [3, 26]. In this vein, one such SDE that has gained recent interest is the so-called Nosé-Hoover equation under Brownian heating (NHB) [6, 23, 27, 38] (see also [37] for related systems). In essence, (NHB) is the usual Langevin system, but it has been augmented by a fictitious control variable.

Compared with the usual Langevin dynamics, the introduction of this auxiliary variable serves a couple of important purposes. First, stochastic gradients can invite noise into the system that is difficult to control [3]. The auxiliary variable is designed to self-correct for this. Second, from a statistical mechanics perspective, existing methods to sample from the canonical measure often fail to keep the system temperature (defined as mean kinetic energy) near a desired value. The new control variable does just this by effectively acting as a thermostat.

While the (NHB) system appears to lead to a desirable dynamical method for sampling from the Gibbs measure in high dimensions, many of the statements made above have only been numerically verified. As an example, it is rigorously known that (NHB) is uniquely ergodic with an explicit stationary distribution whose marginal coincides with canonical distribution [6]. This result holds true in spite of the degenerate nature

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of the equations. Nevertheless, how fast the dynamics approaches stationarity is a practical open problem which is made complicated by the introduction of the thermostat, the very object that leads to the desirable properties above. Intuitively, the auxiliary variable forces the system to large values, and thus how dissipation balances this effect leading to a convergence rate is delicate. In this paper, we solve this open problem by showing that the (NHB) system approaches the augmented Gibbs distribution exponentially fast in an appropriate weighted total variation distance. By integrating out the control variable, the joint position and momentum distribution in turn converges exponentially fast to the canonical Boltzmann-Gibbs measure in a similar sense.

It is important to point out that the main convergence result holds for a wide class of potential functions which we call *normal* below (see Definition 2.1). This class includes the usual polynomial nonlinearities as well as the singular, Lennard-Jones interactions. While the methods of hypocoercivity [4, 7, 8, 10, 12, 16, 33, 43] have proved useful in extracting convergence rates for such potentials in the Langevin dynamics case, we follow the perturbation methods developed in [5, 19, 29] and construct an explicit Lyapunov function. In essence, the type of Lyapunov function exhibited here ensures that return times to large compact sets in space have exponential moments. Thus with the appropriate support and regularity properties of the Markov transitions, geometric convergence to stationarity follows.

The organization of the paper is as follows. In Section 2, we introduce the (NHB) system, fix notation and terminology, and state the main results to be proved in this paper. Section 3 provides heuristic ideas behind the construction of the Lyapunov function. Section 4, Section 5 and the Appendix contain the proofs of the main results.

2. Notation, terminology, and main results

Throughout this paper, we study the following system of SDEs

$$\begin{aligned} dq_i &= \frac{p_i}{m_i} dt \\ dp_i &= -\xi p_i dt - \frac{\gamma}{m_i} p_i dt - \nabla_{q_i} U(q) dt + \sqrt{2\gamma k_B T} dB_i \\ d\xi &= \sum_{i=1}^N \frac{|p_i|^2}{am_i} dt - \frac{k_B T k N}{a} dt. \end{aligned} \tag{NHB}$$

The relations above describe the motion of $N \geq 1$ particles in \mathbf{R}^k with position vector $q = (q_i)_{i=1}^N \in (\mathbf{R}^k)^N$, momentum vector $p = (p_i)_{i=1}^N \in (\mathbf{R}^k)^N$ and mass vector $m = (m_i)_{i=1}^N \in (0, \infty)^N$. Each of the particles is subject to friction ($-\frac{\gamma}{m_i} p_i dt$), thermal fluctuations ($\sqrt{2\gamma k_B T} dB_i$) and a control mechanism $\xi \in \mathbf{R}$, called the *thermostat*, which enacts a friction-like force on the system. The positive parameters k_B, γ, T, a are the Boltzmann, friction, temperature and auxiliary constants, respectively, while the B_i , $i = 1, 2, \dots, N$, are mutually independent standard \mathbf{R}^k -valued Brownian motions defined on a probability space $(\Omega, \mathcal{F}, \mathbf{P}, \mathbf{E})$. The function $U : (\mathbf{R}^k)^N \rightarrow [0, +\infty]$ is the potential, and it encapsulates potential forces on the system as well as any potential interactions between the particles. Throughout, we will assume that U is *normal*, as in the following definition.

DEFINITION 2.1. *We call a function $U : (\mathbf{R}^k)^N \rightarrow [0, +\infty]$ **normal** if it satisfies the following conditions:*

- (A1) *The set $\mathcal{O} = \{q \in (\mathbf{R}^k)^N : U(q) < \infty\}$ is non-empty, open and connected.*

- (A2) For every $n \in \mathbf{N}$, the set $\mathcal{O}_n = \{q \in (\mathbf{R}^k)^N : U(q) < n\}$ has compact closure in $(\mathbf{R}^k)^N$.
- (A3) $U \in C^\infty(\mathcal{O})$ and $\int_{\mathcal{O}} \exp(-\beta U(q)) dq < \infty$ where $\beta := 1/(k_B T)$.
- (A4) There exists a constant $\zeta \in (1, 2)$ such that for any sequence $\{z_n\} \subseteq (\mathbf{R}^k)^N$ with $U(z_n) \rightarrow \infty$ as $n \rightarrow \infty$ we have

$$|\nabla U(z_n)| \rightarrow \infty \text{ and } \frac{|\nabla^2 U(z_n)|}{|\nabla U(z_n)|^\zeta} \rightarrow 0$$

as $n \rightarrow \infty$ where ∇^2 denotes the Hessian operator.

REMARK 2.1. The concept of an *admissible* potential U was introduced in [19] to study relaxation properties of Langevin dynamics under a wide class of potentials. Such a class includes, for example, the Lennard-Jones singular variety. There is however very little difference between the conditions satisfied by an admissible and normal potential; that is, $U : (\mathbf{R}^k)^N \rightarrow [0, +\infty]$ is **admissible** if it satisfies conditions (A1)-(A3) and condition (A4') For any sequence $\{z_n\} \subseteq (\mathbf{R}^k)^N$ with $U(z_n) \rightarrow \infty$ as $n \rightarrow \infty$ we have

$$|\nabla U(z_n)| \rightarrow \infty \text{ and } \frac{|\nabla^2 U(z_n)|}{|\nabla U(z_n)|^2} \rightarrow 0$$

as $n \rightarrow \infty$.

Note that condition (A4') is slightly weaker than (A4) in terms of the asymptotic growth of the Hessian relative to the gradient at large potential energy. Nevertheless, the class of normal potentials is still very wide and includes the usual, polynomial-type potentials as well as the Lennard-Jones singular type. For further discussion as well as specific examples of normal potentials, we refer the reader to Section 4 of [19]. For other works where similar conditions on U were employed, refer to [4, 12, 42].

REMARK 2.2. Note that by setting $m_i = m > 0$ for all i , one can transform the system (NHB) to the associated stochastic Nosé-Hoover systems considered in [6, 23] by making the change of coordinates $\tilde{\xi}(t) = \xi(t) + \gamma/m$. Also, although throughout we restrict ourselves to the case where ξ is real, it is important to point out that it can be matrix-valued. See [6] for further discussion of this point.

For notational simplicity, throughout we let $\mathcal{X} = \mathcal{O} \times (\mathbf{R}^k)^N \times \mathbf{R}$ and use x or (q, p, ξ) to denote a generic point in \mathcal{X} . Similarly, the process solving Equation (NHB) will often be denoted more simply by either $(q(t), p(t), \xi(t))$ or $x(t)$. We let $\mathcal{B}(\mathcal{X})$ denote the Borel σ -field of subsets of \mathcal{X} .

Equation (NHB) has energy functional $H : \mathcal{X} \rightarrow [0, \infty)$ defined by

$$H(q, p, \xi) = \frac{1}{2} \|p\|_m^2 + U(q) + \frac{a\xi^2}{2} \tag{2.1}$$

where

$$\frac{1}{2} \|p\|_m^2 := \frac{1}{2} \sum_i m_i^{-1} |p_i|^2 \tag{2.2}$$

is the kinetic energy. Note that since U satisfies (A3), we may define a probability measure μ on $\mathcal{B}(\mathcal{X})$, called the **augmented Gibbs measure**, by

$$\mu(dq dp d\xi) = \frac{1}{Z} \exp(-\beta H(q, p, \xi)) dr dp d\xi. \tag{2.3}$$

In the above, $\beta = 1/(k_B T)$ and $\mathcal{Z} > 0$ is the normalization constant making μ a probability measure.

We next observe the following lemma giving strong existence and uniqueness of solutions of (NHB).

LEMMA 2.1. *For every initial condition $x \in \mathcal{X}$, Equation (NHB) has unique strong solution $x(t)$ which is defined for all finite times $t \geq 0$ almost surely on the state space \mathcal{X} .*

Lemma 2.1 is an immediate consequence of the main result of this paper (see Theorem 2.2 below), but it can be established more easily by using the energy $H : \mathcal{X} \rightarrow [0, \infty)$ defined in (2.1) as a Lyapunov function. Indeed, by the standard existence and uniqueness theorem for stochastic differential equations, strong solutions of (NHB) are defined and unique until the random time τ_x when the process started from $x \in \mathcal{X}$ exits every set \mathcal{X}_n , $n \in \mathbf{N}$, defined by

$$\mathcal{X}_n = \mathcal{O}_n \times B_n(0) \times (-n, n) \tag{2.4}$$

where $B_n(0)$ denotes the open ball of radius n in $(\mathbf{R}^k)^N$ centered at the origin. Letting

$$\begin{aligned} \mathcal{L} = & \sum_{i=1}^N \frac{p_i}{m_i} \cdot \nabla_{q_i} - \sum_{i=1}^N \left(\xi + \frac{\gamma}{m_i} \right) p_i \cdot \nabla_{p_i} - \nabla U \cdot \nabla_p \\ & + a^{-1} (\|p\|_m^2 - kN/\beta) \partial_\xi + \frac{\gamma}{\beta} \Delta_p \end{aligned}$$

denote the generator of the Markov process (NHB), one can then conclude that $\mathbf{P}\{\tau_x = \infty\} = 1$ for all $x \in \mathcal{X}$ after noting that on \mathcal{X}

$$\begin{aligned} \mathcal{L}H(q, p, \xi) = & -\xi k_B T k N - \gamma \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} + \sum_{i=1}^N \frac{\gamma k_B T}{m_i} \\ \leq & \alpha H(q, p, \xi) + K \end{aligned} \tag{2.5}$$

for some constants $\alpha, K > 0$. That is, the conclusion that $\mathbf{P}\{\tau_x = \infty\} = 1$ for all $x \in \mathcal{X}$ then follows by a standard Gronwall comparison argument, for it implies that $t \mapsto \mathbf{E}_x H(x(t))$ grows no faster than an exponential. See, for example, [17, 25, 32, 35].

REMARK 2.3. For our purposes, the issue with the equality (2.5) is that it does not predict a convergence rate to the presumed equilibrium measure μ . This is because $\mathcal{L}H(q, p, \xi)$ is positive and large when $(q, p, \xi) \in \mathcal{X}$ is such that $\xi \ll -1$ and $|p|$ is bounded. Intuitively, this means that dissipation in the system is not due to pointwise contraction of the H at large energies. Rather, if one expects relaxation to equilibrium, it must be due to averaging effects in the system not captured by the (pointwise) equality (2.5).

By Lemma 2.1, Equation (NHB) induces a Markov semigroup $(\mathcal{P}_t)_{t \geq 0}$ acting on bounded, $\mathcal{B}(\mathcal{X})$ -measurable functions $\varphi : \mathcal{X} \rightarrow \mathbf{R}$ via

$$\mathcal{P}_t \varphi(x) = \mathbf{E}_x \varphi(x(t))$$

for all $t \geq 0$ and dually on probability measures ν on $\mathcal{B}(\mathcal{X})$ by

$$(\nu \mathcal{P}_t)(A) = \int_{\mathcal{X}} \nu(dx) \mathcal{P}_t \mathbf{1}_A(x)$$

for $t \geq 0$ and $A \in \mathcal{B}(\mathcal{X})$. In the above, $\mathbf{1}_A$ denotes the indicator function on the set A . We shall use the notation

$$\mathcal{P}_t(x, A) = \mathcal{P}_t \mathbf{1}_A(x)$$

for $t \geq 0$ and $A \in \mathcal{B}(\mathcal{X})$ to denote the transition probabilities of the Markov process $x(t)$.

We call a probability measure ν on $\mathcal{B}(\mathcal{X})$ an **invariant probability measure** for the Markov process $x(t)$ if $\nu \mathcal{P}_t = \nu$ for all $t \geq 0$. Later, we will see that the augmented Gibbs measure μ in (2.3) is the unique invariant probability measure for $x(t)$. To measure convergence to μ , for $W : \mathcal{X} \rightarrow (0, \infty)$ measurable we let \mathcal{M}_W denote the set of probability measures ν on $\mathcal{B}(\mathcal{X})$ such that $W \in L^1(\nu)$. We equip the set \mathcal{M}_W with a metric $\rho_W : \mathcal{M}_W \times \mathcal{M}_W \rightarrow [0, \infty)$ given by

$$\rho_W(\nu_1, \nu_2) = \sup_{\|\varphi\|_W \leq 1} \int_{\mathcal{X}} \varphi(x) (\nu_1(dx) - \nu_2(dx))$$

where the weighted supremum norm $\|\varphi\|_W$ is defined for measurable $\varphi : \mathcal{X} \rightarrow \mathbf{R}$ by

$$\|\varphi\|_W = \sup_{x \in \mathcal{X}} \frac{|\varphi(x)|}{1 + W(x)}$$

We now state the main result of the paper.

THEOREM 2.1. *We have the following:*

- (a) *The augmented Gibbs measure μ defined in (2.3) is the unique invariant probability measure for the Markov process $x(t)$ solving (NHB).*
- (b) *There exists $\beta_* > 0$ such that for all ϵ, β_0 with $0 < \epsilon < \beta_0 < \beta_*$ there exists $W \in C^2(\mathcal{X}; (0, \infty))$ and constants $C, \eta > 0$ for which*

$$\exp((\beta_0 - \epsilon)H) \leq W \leq \exp((\beta_0 + \epsilon)H)$$

is satisfied on \mathcal{X} and such that the following bound holds for all $\nu \in \mathcal{M}_W$ and all $t \geq 0$

$$\rho_W(\nu \mathcal{P}_t, \mu) \leq C e^{-\eta t} \rho_W(\nu, \mu).$$

As we recall that ξ is a fictitious control variable, consider now the marginal probability distributions $\bar{\mu}$ of μ and $\bar{\mathcal{P}}_t(x, \cdot)$ of $\mathcal{P}_t(x, \cdot)$, $x \in \mathcal{X}$, defined on the Borel sets $\mathcal{B}(\mathcal{Y})$ of $\mathcal{Y} := \mathcal{O} \times (\mathbf{R}^k)^N$ by

$$\bar{\mu}(A) = \sqrt{\frac{2\pi}{\mathcal{Z}^2 a \beta}} \int_A e^{-\beta H(q, p, 0)} dq dp \text{ and } \bar{\mathcal{P}}_t(x, A) = \int_A \int_{\mathbf{R}} \mathcal{P}_t(x, d\xi dq dp)$$

for $A \in \mathcal{B}(\mathcal{Y})$. Note that $\bar{\mu}$ is the canonical Boltzmann-Gibbs measure

$$\bar{\mu}(dq dp) = \sqrt{\frac{2\pi}{\mathcal{Z}^2 a \beta}} \exp(-\beta(\|p\|_m^2/2 + U(q))) dq dp. \tag{2.6}$$

By combining Birkoff's ergodic theorem (see, for example, [35]) with Theorem 2.1, we immediately obtain the following corollary.

COROLLARY 2.1. *For every $f \in L^1(\bar{\mu})$:*

$$\frac{1}{t} \int_0^t f(q(s), p(s)) ds \rightarrow \int_{\mathcal{Y}} f(y) \bar{\mu}(dy) \text{ as } t \rightarrow \infty$$

where the convergence holds μ -almost surely and in the $L^1(\mu)$ -sense. Furthermore, if $W \in C^2(\mathcal{X};(0,\infty))$ is any such function given in the conclusion of Theorem 2.1 and $C, \eta > 0$ are the associated constants in part (b) of the result, then for all $t \geq 0$ and all $x \in \mathcal{X}$ we have

$$\|\overline{\mathcal{P}}_t(x, \cdot) - \bar{\mu}\|_{TV} \leq C e^{-\eta t} \sup_{\|\phi\|_W \leq 1} \left\{ \phi(x) - \int_{\mathcal{X}} \phi(x') \mu(dx') \right\} \tag{2.7}$$

where $\|\cdot\|_{TV}$ denotes the total variation distance.

Before proceeding further, we make some remarks.

REMARK 2.4. In addition to proving Theorem 2.1, we also provide an estimate on the parameter $\beta_* > 0$ in the statement of the result which depends on the maximum, which we will denote by D_{\max} , of Dawson’s integral. Dawson’s integral is a special function $D: \mathbf{R} \rightarrow \mathbf{R}$ defined by

$$D(z) = \exp(-z^2) \int_0^z \exp(y^2) dy \tag{2.8}$$

and it arises in heat conduction and the theory of electrical oscillators [15, 22, 28, 30, 36]. From this point of view, perhaps it is not surprising that it would turn up in the setting of Equation (NHB). To understand why it is surprising from another perspective, later we will see that we can pick

$$\beta_* = \frac{1}{8D_{\max}^2} \beta = 0.42701\dots \times \frac{1}{k_B T} \tag{2.9}$$

and that, to the best of the author’s knowledge, the argument given here does not allow for larger β_* . From working on other stochastic Hamiltonian dynamics, however, one expects to be able to choose $\beta_* = \beta = 1/(k_B T)$ due to the asymptotic behavior of the probability density of the augmented Gibbs measure μ as $H \rightarrow \infty$. Thus from this perspective, there appears to be a discrepancy in the arguments of

$$\beta - \frac{1}{8D_{\max}^2} \beta.$$

The question hence becomes: Is β_* given in (2.9) optimal and if so, why is this the case? In the theoretical arguments that identify the threshold, the behavior of the fictitious control variable ξ in the region where $\xi \ll -1$ and p is bounded plays a fundamental role. Recall from (2.5) that this is the region where the energy of the system is increasing pointwise. We will see that D , hence D_{\max} , is related to the exit distribution of the process from this “bad” part of space, so one might conjecture that D_{\max} is a fundamental parameter governing the stability of the system. Thus the given threshold may not be so surprising.

REMARK 2.5. One can improve the left-hand side of the inequality (2.7) by replacing it with the weighted total variation distance

$$\sup_{\substack{\phi: \mathcal{Y} \rightarrow \mathbf{R} \\ \|\phi\|_W \leq 1}} \int_{\mathcal{Y}} \phi(y) (\overline{\mathcal{P}}_t(x, dy) - \bar{\mu}(dy)) \tag{2.10}$$

where the supremum is taken over all measurable $\phi: \mathcal{Y} \rightarrow \mathbf{R}$ satisfying

$$\sup_{(q,p,\xi) \in \mathcal{X}} \frac{|\phi(q,p)|}{1 + W(q,p,\xi)} \leq 1.$$

Also note that the right-hand side of (2.7) can be made more explicit by bounding it above by

$$Ce^{-\eta t} \left\{ 2 + W(x) + \int_{\mathcal{X}} W(x') \mu(dx') \right\}. \tag{2.11}$$

The proof of Theorem 2.1 splits into two parts: the existence of the appropriate Lyapunov function W to ensure regular and sufficiently fast return times to a compact set in \mathcal{X} , as stated in Theorem 2.2 below, and the necessary support and regularity properties of the Markov transitions outlined in Proposition 2.1.

THEOREM 2.2. *Recall that \mathcal{L} denotes the generator of the Markov process $x(t)$. Let $\epsilon > 0$ and fix $\beta_0 > 0$ satisfying*

$$\beta_0 < \beta_* := \frac{\beta}{8D_{\max}^2}. \tag{2.12}$$

Then there exists $W \in C^2(\mathcal{X})$ and constants $\alpha, K > 0$ such that the following two estimates hold on \mathcal{X}

$$\exp((\beta_0 - \epsilon)H) \leq W \leq \exp((\beta_0 + \epsilon)H), \tag{I}$$

$$\mathcal{L}W \leq -\alpha W + K. \tag{II}$$

The proof of Theorem 2.2 is given in Section 4 and is motivated by the heuristics in Section 3.

Fundamental to the supports of the Markov transitions is the notion of the arc length L_γ of a curve $\gamma \in C^1([0, 1]; \mathcal{O})$ with respect to the norm $\|\cdot\|_m$ defined by

$$L_\gamma = \int_0^1 \|\dot{\gamma}(t)\|_m dt.$$

Since \mathcal{O} is a connected subset of Euclidean space, \mathcal{O} is path connected. Hence this notion of arc length allows us to define the \mathcal{O} -distance $L_{q,q'}$ between $q, q' \in \mathcal{O}$ by

$$L_{q,q'} = \inf \{ L_\gamma : \gamma \in C^1([0, 1]; \mathcal{O}), \gamma(0) = q, \gamma(1) = q' \}.$$

Clearly if $\mathcal{O} = (\mathbf{R}^k)^N$, then $L_{q,q'} = \|q - q'\|_m$. However, if $\mathcal{O} \subsetneq (\mathbf{R}^k)^N$ as in the case of a potential with singularities, then the shortest distance between $q, q' \in \mathcal{O}$ in the norm $\|\cdot\|_m$ is $L_{q,q'}$. For $x = (q, p, \xi) \in \mathcal{X}$ and $t > 0$, define

$$\mathcal{A}(x, t) = \{ (q', p', \xi') \in \mathcal{X} : \xi' \geq \xi + (ta)^{-1} L_{q,q'}^2 - ta^{-1} k_B T k N \}. \tag{2.13}$$

We have the following.

PROPOSITION 2.1.

- (i) *For each $x \in \mathcal{X}$ and $t > 0$, the measure $\mathcal{P}_t(x, \cdot)$ is absolutely continuous with respect to Lebesgue measure on \mathcal{X} . Denoting the probability density of $\mathcal{P}_t(x, \cdot)$ by $r_t(x, y)$, the mapping $(t, x, y) \mapsto r_t(x, y) : (0, \infty) \times \mathcal{X} \times \mathcal{X} \rightarrow [0, \infty)$ is continuous.*
- (ii) *For any $x \in \mathcal{X}$ and $t > 0$*

$$\text{supp } \mathcal{P}_t(x, \cdot) = \mathcal{A}(x, t)$$

where $\text{supp } \nu$ denotes the support of the measure ν and $\mathcal{A}(x, t)$ is as in (2.13).

We will see in the Appendix that Theorem 2.2 and Proposition 2.1 together imply Theorem 2.1. This implication follows from Theorem 1.2 of [14]. In essence, one has to translate the conclusions of Theorem 2.2 and Proposition 2.1 to, respectively, Assumption 1 and Assumption 2 of [14] to an embedded Markov chain. Thus Theorem 1.2 of [14] can be applied to that chain and then one has to translate the bound obtained back to one for the original process, hence producing Theorem 2.1. The proof of Proposition 2.1 relies on by now standard methods to produce the necessary smoothing of the Markov semigroup via Hörmander’s theorem [20] and support properties of the associated transitions via the support theorems [40, 41]. Somewhat surprisingly, in this degenerate setting we are able to produce a characterization (part (ii) of Proposition 2.1) of the supports. The proof of Proposition 2.1 will be given in Section 5.

3. Heuristics

As emphasized at the end of the previous section, the main difficulty in proving Theorem 2.1 is the absence of a natural Lyapunov function. This is clearly evident in Equation (2.5) which shows that $\mathcal{L}H$ is positive and large in the region where $\xi \ll -1$ and $|p|$ is bounded. Thus if we expect dissipation in the system at large energies, then it must be due to averaging effects not captured by the pointwise equality (2.5). As in the works [5, 19], we will look for a small perturbation ψ of the energy H that encapsulates these effects. The construction of such a perturbation uses a slight modification of the procedure developed in [2, 18].

3.1. A simplifying ansatz. Guided by the behavior of the density of μ in (2.3) as $H \rightarrow \infty$, fixing $\epsilon > 0$ and $\beta_0 > 0$ small enough we look for a function $\psi \in C^2(\mathcal{X})$ such that

$$W(x) = \exp(\beta_0 H(x) + \psi(x)) \tag{3.1}$$

satisfies conclusions (I) and (II) of Theorem 2.2. First note that if $V = \beta_0 H + \psi$, then applying the generator \mathcal{L} to W of the form (3.1) produces

$$\mathcal{L}W = W\{\mathcal{L}V + \gamma k_B T |\nabla_p V|^2\}.$$

Thus for this choice of W , conclusion (II) of Theorem 2.2 holds if and only if the following bound holds

$$\mathcal{L}V + \gamma k_B T |\nabla_p V|^2 \leq -\alpha + K \mathbf{1}_A \tag{3.2}$$

on \mathcal{X} for some $\alpha, K > 0$ and $A \subseteq \mathcal{X}$ compact. Note clearly that if the property given in (3.2) holds, then

$$\mathcal{L}V \leq -\alpha + K \mathbf{1}_A \tag{3.3}$$

holds on \mathcal{X} for the same choice of $\alpha, K > 0$ and $A \subseteq \mathcal{X}$ compact. What is surprising is that the reverse implication is often true as well. In other words, by slightly tweaking V satisfying (3.3) we can also obtain the stronger property (3.2), but perhaps for a different choice of α, K, A .

The reverse implication can be intuited by scaling V by a small constant $\epsilon > 0$; that is, if one sets $V_\epsilon = \epsilon V$, then the gradient term in (3.2) is of order ϵ^2 while the $\mathcal{L}V_\epsilon$ is of order ϵ . This also seems plausible when one considers the case when $\psi = 0$, so $V = \beta_0 H$ and hence

$$\mathcal{L}V + \gamma k_B T |\nabla_p V|^2 = \beta_0 \mathcal{L}H + \beta_0^2 \gamma k_B T |\nabla_p H|^2$$

$$= -\gamma\beta_0(1 - \beta_0/\beta) \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \beta_0\xi k_B T k N + \beta_0 \sum_{i=1}^N \frac{\gamma k_B T}{m_i}.$$

Note that as $\beta_0 \searrow 0$, after consulting (2.5) we see that the expression on the right-hand side above is asymptotically equal to $\beta_0\mathcal{L}V$.

With these simple observations in mind, we are now squarely concerned with finding a perturbation ψ so that $V = \beta_0H + \psi$ satisfies the presumably weaker condition (3.3).

3.2. Subsolutions of $\mathcal{L}V = -\alpha$ for $H \gg 1$. Employing our ansatz, fixing $\alpha > 0$ the goal is to now find subsolutions of the PDE

$$\mathcal{L}V = -\alpha \text{ on } H \geq R \tag{3.4}$$

of the form $V = \beta_0H + \psi$ where ψ is the unknown and $R > 0$ is large. Of course, we also want to be able to “tune” the perturbation ψ so that for any $\epsilon > 0$ we can construct $\psi = \psi_\epsilon$ to be a subsolution of (3.4) with the additional property that $|\psi| \leq \epsilon H$ on \mathcal{X} . As we will see below, however, this additional property is a simple consequence of the structure of subsolutions.

We first consult Equation (2.5) to see that in the region

$$\mathcal{R}_0 = \{(q, p, \xi) \in \mathcal{X} : \xi \geq K_* \text{ or } |p|^2 \geq p_* \sqrt{\xi^2 + 1}\}$$

for $K_*, p_* > 0$ sufficiently large we have that

$$\mathcal{L}(\beta_0H) = \beta_0\mathcal{L}H \leq -\alpha.$$

Thus we need not perturb off of the energy to have the desired effect in this region. In other words, we should set

$$\psi = 0 \text{ on } \mathcal{R}_0 \tag{3.5}$$

and restrict our analysis of the problem (3.4) to the complement

$$\mathcal{R}_0^c = \{(q, p, \xi) \in \mathcal{X} : \xi \leq K_* \text{ and } |p|^2 \leq p_* \sqrt{\xi^2 + 1}\}.$$

To help reduce the difficulty in finding subsolutions of (3.4) on \mathcal{R}_0^c , similar to the works [5, 19] we will study the dynamics at large energies. This will be done by using formal scaling analysis applied to the infinitesimal generator

$$\mathcal{L} = \sum_{i=1}^N \frac{p_i}{m_i} \cdot \nabla_{q_i} - \sum_{i=1}^N \left(\xi + \frac{\gamma}{m_i}\right) p_i \cdot \nabla_{p_i} - \nabla U \cdot \nabla_p + a^{-1}(\|p\|_m^2 - kN/\beta) \partial_\xi + \frac{\gamma}{\beta} \Delta_p. \tag{3.6}$$

This analysis allows us to at least heuristically justify neglecting terms in (3.6) when solving (3.4) on \mathcal{R}_0^c . For simplicity, we restrict our discussion in this section to the case when $N = k = m_1 = a = k_B T = 1$, so that

$$\mathcal{L} = p\partial_q - (\xi + \gamma)p\partial_p - U'\partial_p + (p^2 - 1)\partial_\xi + \gamma\partial_p^2. \tag{3.7}$$

Furthermore, to make the scaling analysis that follows more explicit, we will assume that our potential $U : \mathbf{R} \rightarrow [0, \infty)$ is a polynomial of degree $\ell \geq 2$. Note that such a potential satisfies the hypotheses made at the beginning of Section 2.

We start by considering the subregion \mathcal{R}'_1 in \mathcal{R}_0^c where ξ is assumed to be bounded. In particular, $|p|$ must also be bounded in \mathcal{R}'_1 . Consequently, as $H \rightarrow \infty$ in \mathcal{R}'_1 , $U \rightarrow \infty$

while ξ and $|p|$ remain bounded. Thus, making the substitution $q = \lambda Q$ for $\lambda \gg 1$ and not changing ξ and p in the expression (3.7) produces

$$\mathcal{L} = -\lambda^{\ell-1} U'_L(Q) \partial_p + r(Q, p, \xi, \lambda)$$

where U'_L is the leading order term in U' and the remainder term r is $o(\lambda^{\ell-1})$ as $\lambda \rightarrow \infty$. Since $\ell \geq 2$, this argument suggests that in the region \mathcal{R}_0^c where ξ is bounded

$$\mathcal{L} \approx -U'(q) \partial_p. \tag{3.8}$$

A nearly identical scaling argument yields the same approximation (3.8) in the region

$$\mathcal{R}_1 = \mathcal{R}_0^c \cap \{(q, p, \xi) \in \mathcal{X} : |U'(q)| \geq U_*(\xi^6 + 1)^{1/4}\} \tag{3.9}$$

for $U_* > 0$ large enough. Note that the set \mathcal{R}_1 subsumes the region in \mathcal{R}'_1 where H is large. Also, the power $(\xi^6)^{1/4} = |\xi|^{3/2}$ in (3.9) above balances the term $-(\xi + \gamma)p$ on the boundary of \mathcal{R}_0^c where $|p|^2 = p_* \sqrt{\xi^2 + 1}$, so when $U_* > 0$ is large enough, the $-U' \partial_p$ term still dominates.

Translating this scaling analysis back to solving the problem (3.4) in the region \mathcal{R}_1 , we consider solving the equation

$$-U' \partial_p \psi = -\alpha_1 \sqrt{\xi^2 + 1} \tag{3.10}$$

for some constant $\alpha_1 > 0$. Note that the right-hand side of (3.10) is natural since in \mathcal{R}_0^c

$$|\mathcal{L}(\beta_0 H)| \leq C \sqrt{\xi^2 + 1} \tag{3.11}$$

for some $C > 0$. Thus for $\alpha_1 > C$, the solution ψ is designed to counteract any “bad” parts in $\beta_0 \mathcal{L}H$ arising in the region \mathcal{R}_1 . Observe that in \mathcal{R}_1 , Equation (3.10) clearly has a particular solution defined by

$$\psi(q, p, \xi) = \frac{\alpha_1 p \sqrt{\xi^2 + 1}}{U'}, \tag{3.12}$$

thus giving a natural choice for the perturbation ψ in \mathcal{R}_1 . Note that this choice of ψ can be made arbitrarily small on \mathcal{R}_1 by choosing $U_* > 0$ large enough.

We next turn our attention to the region

$$\mathcal{R}_2 = \mathcal{R}_0^c \cap \mathcal{R}_1^c = \{(q, p, \xi) \in \mathcal{X} : \xi \leq K_*, |p|^2 \leq p_* \sqrt{\xi^2 + 1}, |U'| \leq U_*(\xi^6 + 1)^{1/4}\}. \tag{3.13}$$

In \mathcal{R}_2 , any route to infinite energy must have $\xi \rightarrow -\infty$. It is with this fact and how the boundaries in \mathcal{R}_2 for $|p|^2$ and $|U'|$ scale in ξ that we introduce the following family of scaling substitutions:

$$\xi = \lambda \Xi, \quad p = (c_1 \lambda^{1/2} + c_2 + c_3 \lambda^{-\delta})P, \quad q = (c_4 \lambda^{\frac{3}{2(\ell-1)}} + c_5)Q \tag{3.14}$$

where (Q, P, Ξ) are the new variables, and $c_i \in \{0, 1\}$, $\delta > 0$ are constants. Observe that the introduction of the constants $c_i \in \{0, 1\}$ allows us to consider several different scaling regimes. For example if $c_1 = c_3 = c_4 = 0$ and $c_2 = c_5 = 1$, then the scaling transformation in (3.14) becomes $(\xi = \lambda \Xi, p = \lambda^{1/2} P, q = Q)$. Note that this scaling in particular allows us to analyze the part of the region in \mathcal{R}_2 where $|p|^2$ is on the same scale as $|\xi|$ while q remains bounded.

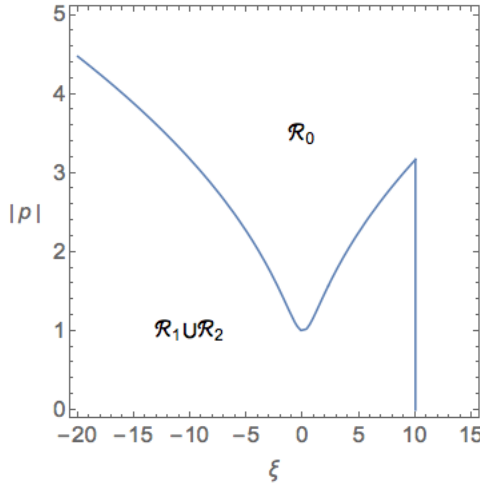


FIG. 3.1. The regions \mathcal{R}_0 and $\mathcal{R}_1 \cup \mathcal{R}_2$ sketched in the $(\xi, |p|)$ -plane with the values $p_* = 1$ and $K_* = 10$.

As dictated by the generator \mathcal{L} , in the region \mathcal{R}_2 we will see that there are four cases covering five qualitatively different scalings. Before we write each of these regimes down, we apply the general transformation (3.14) to the generator to see that in these new coordinates

$$\begin{aligned} \mathcal{L} = & \frac{c_1 \lambda^{1/2} + c_2 + c_3 \lambda^{-\delta}}{c_4 \lambda^{\frac{3}{2(\ell-1)}} + c_5} P \partial_Q - (\lambda \Xi + \gamma) P \partial_P - \frac{U'((c_4 \lambda^{\frac{3}{2(\ell-1)}} + c_5) Q)}{c_1 \lambda^{1/2} + c_2 + c_3 \lambda^{-\delta}} \partial_P \\ & + \lambda^{-1} ((c_1 \lambda^{1/2} + c_2 + c_3 \lambda^{-\delta})^2 - 1) \partial_\Xi + \gamma \frac{1}{(c_1 \lambda^{1/2} + c_2 + c_3 \lambda^{-\delta})^2} \partial_P^2. \end{aligned} \quad (3.15)$$

Case 1. $(c_1 = c_4 = 0, c_2, c_5 = 1, c_3 \in \{0, 1\})$ or $(c_1 = c_5 = 1, c_4 = 0, c_2, c_3 \in \{0, 1\})$. Observe that this is the regime wherein the transformation (3.14) satisfies either $(\xi = \lambda \Xi, p \approx P, q = Q)$ or $(\xi = \lambda \Xi, p \approx \lambda^{1/2} P, q = Q)$. From relation (3.15) we infer that as $\lambda \rightarrow \infty$

$$\mathcal{L} \approx -\lambda \Xi P \partial_P.$$

Case 2. $(c_1 = 0, c_2 = c_4 = 1, c_3, c_5 \in \{0, 1\})$. Recalling that U is a polynomial of degree $\ell \geq 2$ so that U' is a polynomial of degree $\ell - 1$, in this scenario the transformation (3.14) satisfies $(\xi = \lambda \Xi, p \approx P, q \approx \lambda^{\frac{3}{2(\ell-1)}} Q)$. Reading off the dominant balance of terms in (3.15) with this choice of constants, we have that as $\lambda \rightarrow \infty$

$$\mathcal{L} \approx -\lambda^{3/2} U'_L(Q) \partial_P$$

where we recall that U'_L is the leading order term in the polynomial U' .

Case 3. $(c_1 = c_4 = 1, c_2, c_3, c_5 \in \{0, 1\})$. Note that in this case (3.14) satisfies $(\xi = \lambda \Xi, p \approx \lambda^{1/2} P, q \approx \lambda^{\frac{3}{2(\ell-1)}} Q)$. Considering (3.15) in this regime we have that as $\lambda \rightarrow \infty$

$$\mathcal{L} \approx -\lambda \Xi P \partial_P - \lambda U'_L(Q) \partial_P$$

where we neglect any cancellation that could occur between these two leading-order terms.

Case 4. ($c_1 = c_2 = 0, c_3 = 1, c_4, c_5 \in \{0, 1\}$). In this scenario, the scaling (3.14) satisfies ($\xi = \lambda \Xi, p = \lambda^{-\delta} P, q = (c_4 \lambda^{\frac{3}{2(\ell-1)}} + c_5) Q$). This particular case allows us to analyze the dynamics when p is small. From (3.15), it is evident that as $\lambda \rightarrow \infty$

$$\mathcal{L} \approx -\lambda \Xi P \partial_P - \frac{\lambda^\delta}{c_3} U'((c_4 \lambda^{\frac{3}{2(\ell-1)}} + c_5) Q) \partial_P + \frac{\gamma}{c_3^2} \lambda^{2\delta} \partial_P^2.$$

In summary, in the region \mathcal{R}_2 the scaling analysis suggests that at large energies

$$\mathcal{L} \approx \mathcal{A} := -(\xi + \gamma) p \partial_p - U'(q) \partial_p + \gamma \partial_p^2.$$

See Figure 3.1 for a cartoon of the regions $\mathcal{R}_0, \mathcal{R}_1 \cup \mathcal{R}_2$.

REMARK 3.1. Of course we could break apart the region in \mathcal{R}_2 further according to how \mathcal{L} changes above, but the operator \mathcal{A} is simple enough to work with and encapsulates the dominant behaviors identified in the scaling analysis. Note that the reason \mathcal{A} is simple is that the dynamics driven by this operator is constant in ξ and q . In other words, the scalings suggest that in this region at large energies, the Markov process associated to \mathcal{L} is approximated well by the Ornstein-Uhlenbeck dynamics

$$dP_t = -(\xi + \gamma) P_t dt - U'(q) dt + \sqrt{2\gamma} dB_t \tag{3.16}$$

where B_t is a standard, real-valued Brownian motion and $\xi \ll -1$ and $q \in \mathbf{R}$ are fixed constants.

Motivated by this analysis and relation (3.11), for $H \gg 1$ in \mathcal{R}_2 we should take our perturbation ψ to satisfy

$$\mathcal{A} \psi = -\alpha_2 |\xi + \gamma| \tag{3.17}$$

for some constant $\alpha_2 > 0$. Note that in this case we do not need a large negative constant on the right-hand side of the Equation (3.17) because $|\xi| \rightarrow \infty$ at large energies in \mathcal{R}_2 . Also, the appearance of γ in the formula (3.17) does not change the qualitative behavior of the solution but it makes the explicit formula below more compact. Specifically, a particular solution of Equation (3.17) is given by

$$\psi(q, p, \xi) = -2\alpha_2 \int_0^{\frac{|\xi + \gamma|^{1/2}}{\sqrt{2\gamma}} \left(p - \frac{U'(q)}{|\xi + \gamma|} \right)} D(z) dz \tag{3.18}$$

where $D: \mathbf{R} \rightarrow \mathbf{R}$ is Dawson’s integral, which was introduced and discussed in Remark 2.4. By using some well-known asymptotics for the function D , we will see in the next section that for any $\epsilon > 0$, $|\psi(q, p, \xi)| \leq \epsilon H(q, p, \xi)$ in \mathcal{R}_2 for all $|\xi| > 0$ large enough depending on ϵ . Thus using the appropriate cutoff functions, we will see that we can construct, for a given $\epsilon > 0$, our desired subsolution ψ with $|\psi| \leq \epsilon H$ globally.

4. The Lyapunov function

Following the ideas of Section 3, in this section we prove Theorem 2.2. We recall that the Lyapunov function W in the statement of Theorem 2.2 will be of the form (3.1) where H is the energy (2.1) and $\psi \in C^2(\mathcal{X})$ is an appropriately chosen perturbation. The heuristic scaling analysis coupled with the behavior of $\mathcal{L}H(q, p, \xi)$ when $\xi \ll -1$ and $|p|$

is bounded suggested two qualitatively different forms for ψ in two different regions in \mathcal{X} . Refer to expressions (3.12) and (3.18) for these two forms in the simplified case when $N = k = m_1 = a = k_B T = 1$. These forms will be slightly generalized below to account for changes in dimensionality and parameters. We also must cutoff each function when the asymptotic analysis is no longer valid. This will then produce two globally-defined perturbations, which we denote by ψ_1 and ψ_2 below.

REMARK 4.1. We will need one more perturbation, denoted by ψ_0 below, which we did not motivate in the previous section. The function ψ_0 , however, should be thought of as an auxiliary perturbation which places slightly more weight in H on the variable ξ in the region where $\xi < 0$. While a small perturbation itself, it has the advantage of inducing dissipation whenever the kinetic energy is large enough while not changing the essential behavior of $\mathcal{L}(\beta_0 H)$ in the “bad” part of space where $\xi \ll -1$ and $|p|$ is bounded. The function ψ_0 moreover is convenient in that it helps subsume various remainder terms brought on by ψ_1 and ψ_2 .

Following these remarks, Theorem 2.2 is an immediate consequence of the following.

THEOREM 4.1. Fix $\beta_0 > 0$ satisfying (2.12) and $\epsilon \in (0, \beta_0)$. Then there exist $\psi_i \in C^2(\mathcal{X})$, $i = 0, 1, 2$, satisfying the following two properties:

- (i) $|\psi_0 + \psi_1 + \psi_2| \leq \epsilon H$.
- (ii) If $V = \beta_0 H + \psi_0 + \psi_1 + \psi_2$, then there exists a compact set $A \subseteq \mathcal{X}$ and constants $\alpha, K > 0$ for which the bound (3.2) holds.

The proof of Theorem 4.1 will be broken up into several smaller pieces. In particular, as the functions ψ_i are introduced, we will also deduce a series of estimates which, when combined at the end of the section, will imply Theorem 4.1.

4.1. Perturbation ψ_0 . Our first perturbation, ψ_0 , is the simplest. In order to define it, let $f_0 \in C^\infty(\mathbf{R}; [0, 1])$ be a cutoff function satisfying the following conditions

$$f_0(y) = \begin{cases} 1 & \text{if } y \leq -1 \\ 0 & \text{if } y \geq 0 \end{cases}, \quad f'_0 \leq 0, \quad \text{and} \quad |f'_0| \leq 2.$$

Let $\delta > 0$ and for $(q, p, \xi) \in \mathcal{X}$ define

$$\psi_0(q, p, \xi) = \delta f_0(\xi) \frac{a\xi^2}{2}. \tag{4.1}$$

Then it is not hard to check that on \mathcal{X}

$$|\psi_0| \leq \delta H, \tag{4.2}$$

$$\mathcal{L}\psi_0(q, p, \xi) \leq -f_0 \delta |\xi| \|p\|_m^2 + f_0 \frac{\delta}{\beta} k N |\xi| + \frac{\delta}{\beta} k N \tag{4.3}$$

and

$$\nabla_p \psi_0 = 0. \tag{4.4}$$

REMARK 4.2. As discussed in Remark 4.1, note that when $\delta > 0$ in (4.3) is small, ψ_0 allows for a dissipative effect in the region where $\xi \ll -1$ and $\|p\|_m^2$ is bounded below by a sufficiently large positive constant. Moreover, for $\delta > 0$ small, the perturbation is small relative to $\beta_0 H$ and the tradeoff for introducing it is also small relative to $\mathcal{L}(\beta_0 H)$ in the sense that $\mathcal{L}\psi_0 \leq C\delta(|\xi| + 1)$ for some constant $C > 0$ independent of δ .

4.2. Perturbation ψ_1 . Now to define ψ_1 , let $K_* > 0$ be a parameter and $f_i \in C^\infty(\mathbf{R}; [0, 1])$, $i = 1, 2, 3$, be cutoff functions satisfying

$$f_1(y) = \begin{cases} 1 & \text{if } y \leq K_* \\ 0 & \text{if } y \geq K_* + 1 \end{cases}, f_2(y) = \begin{cases} 1 & \text{if } |y| \leq 1 \\ 0 & \text{if } |y| \geq 2 \end{cases}, f_3(y) = \begin{cases} 1 & \text{if } |y| \geq 2 \\ 0 & \text{if } |y| \leq 1 \end{cases}.$$

Let $p_*, U_* > 0$ be parameters and set

$$g_1(q, p, \xi) = f_1(\xi) f_2\left(\frac{|p|^2}{p_* \sqrt{\xi^2 + 1}}\right) f_3\left(\frac{|\nabla U(q)|^2}{U_*(\xi^2 + 1)}\right).$$

Let $\alpha_1 > 0$ and consider ψ_1 defined by

$$\psi_1(q, p, \xi) = \begin{cases} g_1(q, p, \xi) \alpha_1 \sqrt{\xi^2 + 1} \frac{p \cdot \nabla U(q)}{|\nabla U(q)|^2} & \text{if } |\nabla U(q)|^2 \geq U_*/2 \\ 0 & \text{otherwise} \end{cases}. \tag{4.5}$$

Observe that by construction $\psi_1 \in C^\infty(\mathcal{X})$. We will now prove the following.

LEMMA 4.1. *For any $\epsilon, \alpha_1, K_* > 0$, by first picking $p_* > 0$ large enough and then picking $U_* > 0$ large enough we have the global bounds on \mathcal{X}*

$$|\psi_1| \leq \epsilon H, \tag{4.6}$$

$$\mathcal{L}\psi_1 \leq -g_1 \alpha_1 \sqrt{\xi^2 + 1} + \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon |p|^2 + \epsilon f_0 |\xi| + \epsilon, \tag{4.7}$$

$$|\nabla_p \psi_1| \leq \epsilon. \tag{4.8}$$

REMARK 4.3. Note that when $g_1 = 1$, we have

$$\psi_1(q, p, \xi) = \alpha_1 \sqrt{\xi^2 + 1} \frac{p \cdot \nabla U(q)}{|\nabla U(q)|^2} \tag{4.9}$$

and

$$-\nabla U(q) \cdot \nabla_p \psi_1(q, p, \xi) = -\alpha_1 \sqrt{\xi^2 + 1}. \tag{4.10}$$

In particular by setting $N = k = 1$, the function ψ_1 as in (4.9) is precisely the perturbation ψ as in (3.12). Moreover when $g_1 = 1$, ψ_1 satisfies the corresponding version (4.10) of Equation (3.10) in general dimensions.

REMARK 4.4. Note that the region where $g_1 = 1$ does not quite coincide with the form of the region \mathcal{R}_1 introduced in (3.9). In particular, by considering powers of ξ , for large $|\xi|$ the region here is larger than \mathcal{R}_1 in the case when $N = k = 1$. The fact that ψ_1 provides the needed Lyapunov estimate on this larger region is only made possible by the presence of ψ_0 , as it allows us to estimate meddling remainder terms, e.g. $\epsilon |\xi| \|p\|_m^2$ in (4.7), for which ψ_1 itself cannot account. Noticing this fact was crucial in the analysis because it affords the luxury of working with normal, as opposed to a more restricted class of, potentials U .

Proof. (Proof of Lemma 4.1.) The first estimate (4.6) follows easily after noting that

$$|\psi_1(q,p,\xi)| \leq \frac{2\alpha_1 p_*^{1/2}}{U_*^{1/2}} (\xi^2 + 1)^{1/4}.$$

We now turn to the issue of estimating $\mathcal{L}\psi_1$, which we split into three parts as follows

$$\mathcal{L}\psi_1 = \mathcal{T}_1\psi_1 + \mathcal{A}\psi_1 + \mathcal{T}_2\psi_1$$

where $\mathcal{T}_1 = \sum_{i=1}^N m_i^{-1} p_i \cdot \nabla_{q_i}$, $\mathcal{T}_2 = a^{-1}(\|p\|_m^2 - kN/\beta)\partial_\xi$ and

$$\mathcal{A} = \frac{\gamma}{\beta} \Delta_p - \nabla_q U \cdot \nabla_p + \sum_{i=1}^N -\left(\xi + \frac{\gamma}{m_i}\right) p_i \cdot \nabla_{p_i} \tag{4.11}$$

where we again recall that $\beta = 1/(k_B T)$. First note that if $c = \min_i m_i$, then

$$\begin{aligned} \mathcal{T}_1\psi_1 &= \sum_{i,\ell} g_1 \alpha_1 \sqrt{\xi^2 + 1} m_i^{-1} p_i^\ell p \cdot \partial_{q_i^\ell} \left(\frac{\nabla U}{|\nabla U|^2} \right) \\ &\quad + \sum_{i,\ell,j,\ell'} f_1 f_2 f_3' \alpha_1 \sqrt{\xi^2 + 1} m_i^{-1} p_i^\ell p \cdot \nabla U \frac{2(\partial_{q_j^{\ell'}} U) \partial_{q_i^\ell q_j^{\ell'}} U}{|\nabla U|^2 U_* (\xi^2 + 1)} \\ &\leq g_1 c^{-1} \alpha_1 \sqrt{\xi^2 + 1} |p|^2 |\nabla G| + 4c^{-1} f_1 f_2 |f_3'| \alpha_1 \sqrt{\xi^2 + 1} |p|^2 \frac{|\nabla^2 U|}{|\nabla U|^2} \end{aligned}$$

where $G = \nabla U / |\nabla U|^2$. Note that for every $\epsilon, \alpha_1, K_* > 0$ since U is a normal potential (see Definition 2.1) we may choose $U_* > 0$ large enough to control the ∇G and $|\nabla^2 U| / |\nabla U|^2$ terms above and arrive at the global estimate

$$\mathcal{T}_1\psi_1(q,p,\xi) \leq \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon |p|^2. \tag{4.12}$$

Turning to the next term $\mathcal{A}\psi_1$, observe that

$$\begin{aligned} \mathcal{A}\psi_1 &= \frac{4\gamma\alpha_1 + 2\gamma\alpha_1 kN}{\beta p_*} f_1 f_2' f_3 \frac{p \cdot \nabla U}{|\nabla U|^2} + \frac{4\gamma\alpha_1}{\beta p_*} f_1 f_2'' f_3 \frac{|p|^2}{p_* \sqrt{\xi^2 + 1}} \frac{p \cdot \nabla U}{|\nabla U|^2} \\ &\quad - g_1 \alpha_1 \sqrt{\xi^2 + 1} + \frac{2\alpha_1}{p_*} f_1 f_2' f_3 \frac{(p \cdot \nabla U)^2}{|\nabla U|^2} \\ &\quad + \sum_{i=1}^N -g_1 \alpha_1 (\xi + \gamma/m_i) \sqrt{\xi^2 + 1} \frac{p_i \cdot \nabla_{q_i} U}{|\nabla U|^2} \\ &\quad + \sum_{i=1}^N -\frac{2\alpha_1}{p_*} f_1 f_2' f_3 (\xi + \gamma/m_i) |p_i|^2 \frac{p \cdot \nabla U}{|\nabla U|^2}. \end{aligned}$$

Recalling that $c = \min_i m_i > 0$, note that we can estimate each term above as follows

$$\begin{aligned} \mathcal{A}\psi_1 &\leq -g_1 \alpha_1 \sqrt{\xi^2 + 1} + \frac{4\gamma\alpha_1 + 2\gamma\alpha_1 kN}{\beta p_*} f_1 |f_2'| f_3 \frac{|p|}{|\nabla U|} \\ &\quad + \frac{8\gamma\alpha_1}{\beta p_*} f_1 |f_2''| f_3 \frac{|p|}{|\nabla U|} + \frac{2\alpha_1}{p_*} f_1 |f_2'| f_3 |p|^2 \end{aligned}$$

$$+ g_1 \alpha_1 \frac{(|\xi| + \gamma/c) \sqrt{\xi^2 + 1}}{|\nabla U|} |p| + \frac{2\alpha_1}{p_*} f_1 |f'_2| f_3 \frac{(|\xi| + \gamma/c) |p|}{|\nabla U|} |p|^2.$$

Now for any $\epsilon, \alpha_1, K_* > 0$, by first picking $p_* > 0$ large enough and then picking $U_* > 0$ large enough, we arrive at the global estimate

$$\mathcal{A} \psi_1 \leq -g_1 \alpha_1 \sqrt{\xi^2 + 1} + \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon f_0 |\xi| + \epsilon |p|^2 + \epsilon. \tag{4.13}$$

Finally, we estimate $\mathcal{T}_2 \psi_1$. Note that

$$\begin{aligned} \mathcal{T}_2 \psi_1(q, p, \xi) &= \frac{\alpha_1 p \cdot \nabla U}{a |\nabla U|^2} (\|p\|_m^2 - kN/\beta) \left\{ f'_1 f_2 f_3 \sqrt{\xi^2 + 1} - f_1 f'_2 f_3 \frac{|p|^2 \xi}{p_* (\xi^2 + 1)} \right. \\ &\quad \left. - f_1 f_2 f'_3 \frac{2|\nabla U|^2 \xi}{U_* (\xi^2 + 1)^{3/2}} + g_1 \frac{\xi}{\sqrt{\xi^2 + 1}} \right\} \\ &\leq (\|p\|_m^2 + kN/\beta) \left\{ \frac{\alpha_1}{a} |f'_1| f_2 f_3 \frac{|p| \sqrt{\xi^2 + 1}}{|\nabla U|} + \frac{2\alpha_1}{a} f_1 |f'_2| f_3 \frac{|p| |\xi|}{|\nabla U| \sqrt{\xi^2 + 1}} \right. \\ &\quad \left. + \frac{4\alpha_1}{a} f_1 f_2 |f'_3| \frac{|p| |\xi|}{|\nabla U| (\xi^2 + 1)} + \frac{\alpha_1}{a} \frac{|p| |\xi|}{|\nabla U| \sqrt{\xi^2 + 1}} \right\}. \end{aligned}$$

Thus by counting powers of $|\xi|$, for any choice of $\epsilon, \alpha_1, p_*, K_* > 0$, we may pick $U_* > 0$ large enough so that

$$\mathcal{T}_2 \psi_1(q, p, \xi) \leq \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon f_0 |\xi| + \epsilon |p|^2 + \epsilon. \tag{4.14}$$

Combining the bounds (4.12), (4.13) and (4.14) and adjusting $\epsilon > 0$ and the constants appropriately produces the estimate (4.7).

To establish the bound on $\nabla_p(\psi_1)$ observe that

$$\nabla_p \psi_1 = g_1 \alpha_1 \sqrt{\xi^2 + 1} \frac{\nabla U}{|\nabla U|^2} + f_1 f'_2 f_3 \frac{2\alpha_1 p \cdot \nabla U}{p_* |\nabla U|^2},$$

hence

$$|\nabla_p \psi_1| \leq g_1 \alpha_1 \frac{\sqrt{\xi^2 + 1}}{|\nabla U|} + f_1 |f'_2| f_3 \frac{2\alpha_1 |p|^2}{p_* |\nabla U|}.$$

Thus for every $\epsilon, \alpha_1, p_*, K_* > 0$ we may pick $U_* > 0$ large enough so that the estimate (4.8) holds. □

4.3. Perturbation ψ_2 . In order to define the second perturbation ψ_2 , let $\alpha_2 > 0$ be a parameter and $F: \mathbf{R} \rightarrow \mathbf{R}$ be given by

$$F(z) = -2\alpha_2 \int_0^z \exp(-y^2) \int_0^y \exp(x^2) dx dy. \tag{4.15}$$

Observe that $F'/(-2\alpha_2) = D$ where D is Dawson’s integral, as defined and discussed in Remark 2.4. The function F will make up part of the formula for ψ_2 , and thus we will need the following proposition in our analysis below.

PROPOSITION 4.1. *As $|z| \rightarrow \infty$*

$$\frac{|F(z)|}{\alpha_2 \log(|z|)} \rightarrow 1 \quad \text{and} \quad \frac{|z| |F'(z)|}{\alpha_2} \rightarrow 1. \tag{4.16}$$

Proof. By symmetry, it suffices to prove the asymptotic formulas as $z \rightarrow \infty$. Note that for $z \geq 1$ we may write

$$-\frac{F(z)}{2\alpha_2} = \int_1^z \exp(-y^2) \int_1^y \exp(x^2) dx dy + R_0(z) \tag{4.17}$$

where

$$R_0(z) = \int_0^1 \exp(-y^2) \int_0^y \exp(x^2) dx dy + \int_1^z \exp(-y^2) \int_0^1 \exp(x^2) dx dy$$

satisfies $R_0(z) = o(\log(z))$ and $R'_0(z) = o(1/z)$ as $z \rightarrow \infty$. After writing

$$\int_1^y \exp(x^2) dx = \int_1^y \frac{1}{2x} (\exp(x^2))' dx$$

integration by parts on this term in (4.17) produces

$$-\frac{F(z)}{2\alpha_2} = \frac{\log(z)}{2} + R_0(z) + R_1(z)$$

where

$$R_1(z) = - \int_1^z \exp(-y^2) dy + \int_1^z \exp(-y^2) \int_1^y \frac{\exp(x^2)}{2x^2} dx dy$$

also satisfies $R_1(z) = o(\log(z))$ and $R'_1(z) = o(1/z)$ as $z \rightarrow \infty$. This finishes the proof. \square

Fix $i \in \{1, 2, \dots, N\}$ and a constant $\xi_* > \max_j (3\gamma/m_j + 1)$. Let $h_2 = f_2$ and introduce auxiliary cutoff functions $h_i \in C^\infty(\mathbf{R}; [0, 1])$, $i = 1, 3$, satisfying

$$h_1(y) = \begin{cases} 1 & \text{if } y \leq -\xi_* - 1 \\ 0 & \text{if } y \geq -\xi_* \end{cases} \quad \text{with} \quad |h'_1| \leq 2$$

and

$$h_3(y) = \begin{cases} 1 & \text{if } |y| \leq 3 \\ 0 & \text{if } |y| \geq 4 \end{cases}$$

Recalling the parameters $p_*, U_* > 0$, define

$$g_2(q, p, \xi) = h_1(\xi) h_2\left(\frac{|p|^2}{p_* \sqrt{\xi^2 + 1}}\right) h_3\left(\frac{|\nabla U(q)|^2}{U_*(\xi^2 + 1)}\right).$$

Fixing $\ell \in \{1, 2, \dots, k\}$ we set

$$\psi_i^\ell(q, p, \xi) = \begin{cases} g_2(q, p, \xi) F\left(\frac{|\xi + \frac{\gamma}{m_i}|^{1/2}}{\sqrt{2\gamma/\beta}} \left(p_i^\ell - \frac{\partial_{q_i} U}{|\xi + \frac{\gamma}{m_i}|}\right)\right) & \text{if } \xi \leq -\frac{3\gamma}{m_i} \\ 0 & \text{if } \xi > -\frac{3\gamma}{m_i} \end{cases}$$

and define $\psi_2 : \mathcal{X} \rightarrow \mathbf{R}$ by

$$\psi_2(q, p, \xi) = \sum_{i=1}^N \sum_{\ell=1}^k \psi_i^\ell(q, p, \xi). \tag{4.18}$$

Our next goal is to prove the following:

LEMMA 4.2. *For each $\epsilon, \alpha_2, K_* > 0$ we can pick $p_* > 0$ large enough, then $U_* > 0$ large enough and then $\xi_* > 0$ large such that the following estimates hold on \mathcal{X}*

$$|\psi_2| \leq \epsilon H, \tag{4.19}$$

$$\mathcal{L}\psi_2(q, p, \xi) \leq -\alpha_2 k N g_2 |\xi| + \epsilon |p|^2 + \epsilon + \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon f_0 |\xi|, \tag{4.20}$$

and

$$\frac{\gamma}{\beta} |\nabla_p(\psi_2)|^2 \leq 2k N \alpha_2^2 D_{\max}^2 g_2 |\xi| + \epsilon f_0 |\xi| + \epsilon. \tag{4.21}$$

REMARK 4.5. To compare with the heuristics of Section 3, note that if $g_2 = 1$ we have $\xi \leq -3\gamma/m_i$ for every i for $\xi_* > 0$ large enough. Thus when $N = k = m_1 = a = k_B T = 1$, ψ_2 above precisely coincides with ψ in (3.18), which we recall is a particular solution of the Equation (3.17). Now observe that ψ_i^ℓ is the corresponding particular solution of the equation

$$\mathcal{A}_i^\ell \psi_i^\ell(q, p, \xi) = -\alpha_2 |\xi + \gamma/m_i|.$$

where

$$\mathcal{A}_i^\ell = (|\xi + \gamma/m_i| p_i^\ell - \partial_{q_i^\ell} U) \partial_{p_i^\ell} + \frac{\gamma}{\beta} \partial_{p_i^\ell}^2. \tag{4.22}$$

Hence when $g_2 = 1$, ψ_2 is simply the superposition of these particular solutions. Heuristically this makes sense since at large energies where $g_2 \neq 0$, ξ and q are approximately constant so that each momentum variable p_i^ℓ is “approximately” independent.

Proof. (Proof of Lemma 4.2.) To see the first estimate (4.19), fix $i \in \{1, 2, \dots, N\}$ and $\ell \in \{1, 2, \dots, k\}$. Applying Proposition 4.1, we see that there exist constants $C, D > 0$ such that for all $(q, p, \xi) \in \mathcal{X}$

$$|\psi_i^\ell(q, p, \xi)| \leq g_2 (C \log |\xi| + D).$$

Since $0 \leq g_2 \leq 1$ globally and $g_2 \equiv 0$ whenever $\xi \geq -\xi_*$, it follows that we may pick $\xi_* > 0$ large enough so that (4.19) holds.

To estimate $\mathcal{L}\psi_2$, we again fix $i \in \{1, 2, \dots, N\}$ and $\ell \in \{1, 2, \dots, k\}$ and estimate $\mathcal{L}\psi_i^\ell$, showing that for each $\epsilon, \alpha_2, K_* > 0$, we may pick $p_* > 0$ large enough, then $U_* > 0$ large enough and then $\xi_* > 0$ large enough so that the estimate

$$\mathcal{L}\psi_i^\ell(q, p, \xi) \leq -\alpha_2 g_2 |\xi| + \epsilon |p|^2 + \epsilon + \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon f_0 |\xi| \tag{4.23}$$

holds on \mathcal{X} . As in the previous lemma, we again break up $\mathcal{L}\psi_i^\ell$ as

$$\mathcal{L}\psi_i^\ell = \mathcal{T}_1 \psi_i^\ell + \mathcal{A} \psi_i^\ell + \mathcal{T}_2 \psi_i^\ell$$

where $\mathcal{T}_1, \mathcal{T}_2$ and \mathcal{A} were introduced either just above or in Equation (4.11). Even though F in the definition of ψ_i^ℓ depends on i, ℓ , we will suppress this dependence for simplicity. Beginning with $\mathcal{T}_1 \psi_i^\ell$ observe that if $c = \min_i m_i$ we have

$$\mathcal{T}_1 \psi_i^\ell = \sum_{n,j} \left\{ -g_2 F' \frac{p_n^j \partial_{q_n^j}^2 U}{\sqrt{2\gamma/\beta} |\xi + \gamma/m_i|} + \sum_{s,t} h_1 h_2 h_3 F \frac{2p_n^j \partial_{q_s^j} U \partial_{q_n^t}^2 U}{U_* (\xi^2 + 1)} \right\} \frac{1}{m_n}$$

$$\begin{aligned} &\leq c^{-1}g_2 \frac{|F'|\|p\|\nabla^2U|}{\sqrt{2\gamma/\beta|\xi+\gamma/m_i|}} + 2c^{-1}h_1h_2|h'_3| \frac{|F|\|\nabla U\|\nabla^2U\|p|}{U_*(\xi^2+1)} \\ &\leq c^{-1}g_2 \frac{|F'|\|p\|\nabla^2U|}{\sqrt{2\gamma/\beta|\xi+\gamma/m_i|}} 1_{\{U\leq R\}} + c^{-1}g_2 \frac{|F'|\|p\|\nabla U|^\zeta}{\sqrt{2\gamma/\beta|\xi+\gamma/m_i|}} \frac{|\nabla^2U|}{|\nabla U|^\zeta} 1_{\{U\geq R\}} \\ &\quad + 2c^{-1}h_1h_2|h'_3| \frac{|F|\|\nabla U\|\nabla^2U\|p|}{U_*(\xi^2+1)} 1_{\{U\leq R\}} \\ &\quad + 4c^{-1}h_1h_2|h'_3| |F|\|\nabla U\|^{\zeta-1}|p| \frac{|\nabla^2U|}{|\nabla U|^\zeta} 1_{\{U\geq R\}} \end{aligned}$$

where $\zeta \in (1, 2)$ is the constant in (A4) of Definition 2.1. Applying the asymptotics in (A4) and those for F in Proposition 4.1, for each $\epsilon > 0$ we may pick $R > 0$ large enough so that

$$\mathcal{T}_1\psi_i^\ell \leq C_1g_2 \frac{|p|}{|\xi+\gamma/m_i|^{1/2}} + \epsilon g_2|p|\|\xi\|^{1/2} + 2C_2h_1h_2|h'_3| \frac{|p|}{|\xi|} + \epsilon h_1h_2|h'_3|\|\xi\||p|$$

for some constants $C_i > 0$ depending on $\alpha_2, p_*, U_*, \epsilon, R$. Thus for all $\epsilon, \alpha_2, p_*, U_* > 0$, picking $\xi_* > 0$ large enough we can arrive at the inequality

$$\mathcal{T}_1\psi_i^\ell \leq \epsilon + \epsilon f_0|\xi| + \epsilon f_0|\xi|\|p\|_m^2. \tag{4.24}$$

Turning now to $\mathcal{A}\psi_i^\ell$, recall the definition of \mathcal{A}_i^ℓ given in (4.22) and note

$$\begin{aligned} \mathcal{A}\psi_i^\ell &= \mathcal{A}_i^\ell\psi_i^\ell + \sum_{(n,j)\neq(i,\ell)} F\mathcal{A}_n^jg_2 \\ &= g_2\mathcal{A}_i^\ell(F) + \frac{2\gamma}{\beta}\partial_{p_i^\ell}(g_2)\partial_{p_i^\ell}(F) + \sum_{n,j} F\mathcal{A}_n^jg_2 \\ &= -\alpha_2g_2|\xi+\gamma/m_i| + \sqrt{2\gamma/\beta}h_1h_2h_3F' \frac{2p_i^\ell|\xi+\gamma/m_i|^{1/2}}{p_*\sqrt{\xi^2+1}} + \sum_{n,j} F\mathcal{A}_n^jg_2. \end{aligned}$$

Now,

$$\begin{aligned} F\mathcal{A}_n^jg_2 &= Fh_1h_2h_3 \frac{2p_n^j}{p_*\sqrt{\xi^2+1}} (|\xi+\gamma/m_n|p_n^j - \partial_{q_n^j}U) + \frac{\gamma}{\beta}Fh_1h_2h_3 \frac{4(p_n^j)^2}{p_*^2(\xi^2+1)} \\ &\quad + \frac{\gamma}{\beta}Fh_1h_2h_3 \frac{2}{p_*\sqrt{\xi^2+1}} \\ &\leq C_1h_1|h'_2|h_3\|p\|\xi+\gamma/m_n\|^{1/2} \log|\xi+\gamma| + C_2(h_1|h'_2|h_3+h_1|h_2''|h_3) \frac{\log|\xi+\gamma/m_n|}{\sqrt{\xi^2+1}} \end{aligned}$$

for some constants $C_i > 0$ depending on α_2, p_*, U_* . Thus for every $\epsilon, \alpha_2, p_*, U_*, K_* > 0$, picking $\xi_* > 0$ large enough produces the global estimate

$$\mathcal{A}\psi_i^\ell \leq -\alpha_2g_2|\xi| + \epsilon f_0\|p\|_m^2|\xi| + \epsilon f_0|\xi| + \epsilon|p|^2 + \epsilon. \tag{4.25}$$

Lastly, we consider $\mathcal{T}_2\psi_i^\ell$ and note

$$\mathcal{T}_2\psi_i^\ell = a^{-1}(\|p\|_m^2 - kNk_B T) \times \left\{ h'_1h_2h_3F - h_1h_2h_3F \frac{\xi|p|^2}{p_*^2(\xi^2+1)^{3/2}} \right.$$

$$\begin{aligned}
 & -2h_1h_2h_3F \frac{\xi|\nabla U|^2}{U_*(\xi^2+1)^2} + \frac{g_2}{2|\xi+\gamma/m_i|} F' \frac{|\xi+\gamma/m_i|^{1/2}}{\sqrt{2\gamma/\beta}} \left(p_i^m - \frac{\partial_{q_i^\ell} U}{|\xi+\gamma/m_i|} \right) \\
 & \left. + \frac{g_2 F' \partial_{q_i^\ell} U}{\sqrt{2\gamma/\beta} |\xi+\gamma/m_i|^{3/2}} \right\}.
 \end{aligned}$$

Hence,

$$\begin{aligned}
 \mathcal{T}_2 \psi_\ell^m \leq a^{-1} (\|p\|_m^2 + kNk_B T) & \left\{ |h'_1| h_2 h_3 |F| + 2h_1 |h'_2| h_3 \frac{|\xi|}{\xi^2+1} + 6h_1 h_2 |h'_3| \frac{|\xi|}{\xi^2+1} \right. \\
 & \left. + C_1 \frac{g_2}{|\xi+\gamma/m_\ell|} + C_2 g_2 \right\}
 \end{aligned}$$

for some constant $C_1 > 0$ depending on α_2 and some constant $C_2 > 0$ depending on α_2, U_* . Picking $\xi_* > 0$ large enough as before, we can thus arrive at the estimate

$$\mathcal{T}_2 \psi_i^\ell \leq \epsilon f_0 |\xi| \|p\|_m^2 + \epsilon f_0 |\xi|. \tag{4.26}$$

Putting the estimates together we arrive at the claimed inequality (4.23).

Finally, we turn to estimating $\frac{2}{\beta} |\nabla_p(\psi_2)|^2$. Note that for each $i, j \in \{1, 2, \dots, N\}$ and each $n, \ell \in \{1, 2, \dots, k\}$ we have that

$$\partial_{p_j^n}(\psi_i^\ell) = \delta_{(i,\ell)}(j,n) g_2 F' \frac{|\xi+\gamma/m_i|^{1/2}}{\sqrt{2\gamma/\beta}} + h_1 h'_2 h_3 F \frac{2p_j^n}{p_* \sqrt{\xi^2+1}}$$

where $\delta_{(i,\ell)}(j,n) = 1$ if $(j,n) = (i,\ell)$ and 0 otherwise. Hence

$$|\partial_{p_j^n}(\psi_2)| \leq g_2 \frac{2\alpha_2 D_{\max}}{\sqrt{2\gamma/\beta}} |\xi+\gamma/m_j|^{1/2} + h_1 |h'_2| h_3 \frac{4(C \log |\xi| + D)}{p_*^{1/2} (\xi^2+1)^{1/4}}$$

for some constants $C, D > 0$. Thus applying Proposition 4.1 for every $\epsilon > 0$ by picking $\xi_* > 0$ large as before we find that

$$|\partial_{p_j^n}(\psi_2)| \leq g_2 \frac{2\alpha_2 D_{\max}}{\sqrt{2\gamma/\beta}} |\xi+\gamma/m_j|^{1/2} + \epsilon$$

for all j, n . Hence applying this bound and by possibly increasing $\xi_* > 0$ if necessary we arrive at the claimed estimate (4.21). \square

We now combine the previous estimates to prove Theorem 4.1. Whenever we need to adjust the parameters as done in the statement of Lemma 4.2, in the proof below we will simply say “by adjusting the parameters”. Also, we have provided a sketch of the basic form of the Lyapunov function $V = \beta_0 H + \psi_0 + \psi_1 + \psi_2$ in Figure 4.1 in various regions in the $(\xi, |p|)$ -plane.

Proof. (Proof of Theorem 4.1.) Let $\beta_0 > 0$ satisfy (2.12) and fix $\epsilon_0 \in (0, \beta_0)$. Pick $\delta > 0$ such that

$$\delta = \min \left\{ \frac{\epsilon_0}{3}, \frac{\beta_*}{2} - \frac{\beta_0}{2} \right\}$$

where we recall the constant $\delta > 0$ was introduced above (4.1). Note that by adjusting the parameters, the estimates (4.2), (4.6) and (4.19) together imply part (i) of the result.

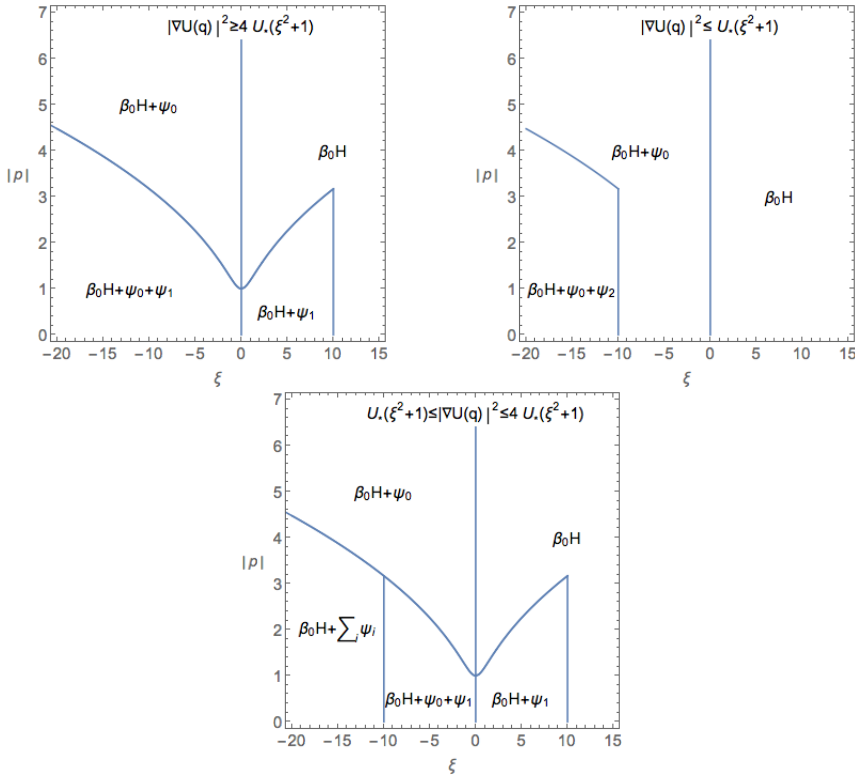


FIG. 4.1. The form of the Lyapunov function $V = \beta_0 H + \psi_0 + \psi_1 + \psi_2$ given in the $(\xi, |p|)$ -plane for $|\nabla U|^2 \geq 4U_*(\xi^2 + 1)$, $|\nabla U|^2 \leq U_*(\xi^2 + 1)$ and $U_*(\xi^2 + 1) \leq |\nabla U|^2 \leq 4U_*(\xi^2 + 1)$, respectively. For simplicity, here we have chosen $K_* + 1 = \xi_* + 1 = 10$ and $p_* = 1/2$.

To establish condition (ii) of the result, first note that

$$\mathcal{L}(\beta_0 H) = -\gamma \beta_0 \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \frac{\beta_0}{\beta} k N \xi + \frac{\beta_0}{\beta} K_1, \tag{4.27}$$

where $K_1 := \gamma \sum_i m_i^{-1} > 0$, and

$$\nabla_{p_i}(\beta_0 H) = \beta_0 \frac{p_i}{m_i}. \tag{4.28}$$

Let $V = \beta_0 H + \psi_0 + \psi_1 + \psi_2$. Combining relations (4.3) and (4.4) with Lemma 4.1 and Lemma 4.2, for each $\epsilon > 0$ we may vary the parameters so that

$$\begin{aligned} \mathcal{L}V(q, p, \xi) &\leq -\gamma \beta_0 (1 - \epsilon) \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \frac{\beta_0}{\beta} k N \xi - f_0 \delta (1 - \epsilon) |\xi| \|p\|_m^2 \\ &\quad - g_1 \alpha_1 \sqrt{\xi^2 + 1} - \alpha_2 k N g_2 |\xi| + f_0 \frac{\delta + \epsilon}{\beta} k N |\xi| + \frac{\beta_0}{\beta} K_1 + \frac{\delta + \epsilon}{\beta} k N \end{aligned} \tag{4.29}$$

as well as the inequality

$$\frac{\gamma}{\beta} |\nabla_p V|^2 \leq \frac{\gamma}{\beta} \left\{ |\nabla_p(\beta_0 H)|^2 + |\nabla_p(\psi_1)|^2 + |\nabla_p(\psi_2)|^2 + 2|\nabla_p(\beta_0 H)||\nabla_p(\psi_1)| \right\}$$

$$\begin{aligned}
 &+ 2|\nabla_p(\beta_0 H)||\nabla_p(\psi_2)| + 2|\nabla_p(\psi_1)||\nabla_p(\psi_2)| \Big\} \\
 &\leq \frac{\gamma\beta_0^2}{\beta} \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} + 2kN\alpha_2^2 D_{\max}^2 |\xi| + \epsilon f_0 |\xi| + \epsilon f_0 \|p\|_m^2 |\xi| + \epsilon + \epsilon |p|^2.
 \end{aligned}$$

Combining the previous inequality with (4.29) and adjusting $\epsilon > 0$ and the parameters accordingly produces the estimate

$$\begin{aligned}
 &\mathcal{L}V(q, p, \xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 \\
 &\leq -\gamma\beta_0(1 - \beta_0/\beta - \epsilon) \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \frac{\beta_0}{\beta} kN\xi - f_0\delta(1 - \epsilon)|\xi| \|p\|_m^2 \\
 &\quad - g_1\alpha_1\sqrt{\xi^2 + 1} - g_2\alpha_2 kN(1 - 2\alpha_2 D_{\max}^2) |\xi| + f_0 \frac{\delta + \epsilon}{\beta} kN |\xi| + \frac{\beta_0}{\beta} K_1 + \frac{\delta + \epsilon}{\beta} kN. \tag{4.30}
 \end{aligned}$$

Let $\alpha > 0$ and pick the rest of the parameters as follows:

$$\epsilon < \min \left\{ \frac{1}{2} - \frac{\beta_0}{2\beta}, \frac{1}{2}, \frac{\beta}{8D_{\max}^2} - \beta_0 - \delta \right\}, \quad \alpha_1 = 2\alpha + 2\frac{\beta_0}{\beta} K_1 + 2\frac{\beta_0 + \delta + \epsilon}{\beta} kN, \tag{4.31}$$

$$\alpha_2 = \frac{1}{4D_{\max}^2} \quad K_* = \frac{\beta\alpha}{\beta_0 kN} + \frac{K_1}{kN} + \frac{\beta_0 + \delta + \epsilon}{\beta_0}. \tag{4.32}$$

Applying these choices to the estimate (4.30) then gives

$$\begin{aligned}
 \mathcal{L}V(q, p, \xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 &\leq -\frac{\gamma\beta_0}{2}(1 - \beta_0/\beta) \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \frac{\beta_0}{\beta} kN |\xi| (1 - f_0) - \frac{f_0}{2} \delta |\xi| \|p\|_m^2 \\
 &\quad - g_1 \frac{\alpha_1}{2} |\xi| - g_1 \frac{\alpha_1}{2} - g_2 \frac{kN}{8D_{\max}^2} |\xi| + f_0 \frac{\beta_0 + \delta + \epsilon}{\beta} kN |\xi| \\
 &\quad + \frac{\beta_0}{\beta} K_1 + \frac{\beta_0 + \delta + \epsilon}{\beta} kN
 \end{aligned}$$

where we have left α_1 as is for brevity of mathematical expression. First observe that if $\xi \geq K_*$, then

$$\mathcal{L}V(q, p, \xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 \leq -\frac{\beta_0}{\beta} kN K_* + \frac{\beta_0}{\beta} K_1 + \frac{\beta_0 + \delta + \epsilon}{\beta} kN \leq -\alpha.$$

Also note that

$$\begin{aligned}
 \mathcal{L}V(q, p, \xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 &\leq -\frac{\gamma\beta_0}{2}(1 - \beta_0/\beta) \sum_{i=1}^N \frac{|p_i|^2}{m_i^2} - \frac{f_0}{2} \delta |\xi| \|p\|_m^2 \\
 &\quad + f_0 \frac{\beta_0 + \delta + \epsilon}{\beta} kN |\xi| + \frac{\beta_0}{\beta} K_1 + \frac{\beta_0 + \delta + \epsilon}{\beta} kN.
 \end{aligned}$$

Hence if $c = \min_i m_i$ and $|p| \geq P > 0$ for any $P > 0$ sufficiently large we have

$$\mathcal{L}V(q, p, \xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 \leq -\alpha.$$

Thus now suppose that $|p| \leq P$ and $-\xi_* - 3 \leq \xi \leq K_*$. This means that both $|p|$ and ξ are bounded. Thus the only possibility for $H \rightarrow \infty$ is if $U(q) \rightarrow \infty$. Thus, for $U(q)$ large enough in this region, $g_1 = 1, f_0 = 1$ and

$$\begin{aligned} \mathcal{L}V(q,p,\xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 &\leq -\frac{\alpha_1}{2} |\xi| - \frac{\alpha_1}{2} + \frac{\beta_0 + \delta + \epsilon}{\beta} kN |\xi| + \frac{\beta_0}{\beta} K_1 + \frac{\beta_0 + \delta + \epsilon}{\beta} kN \\ &\leq -\alpha \end{aligned}$$

where in the last inequality we used the choice of α_1 in (4.31). Finally, if $|p| \leq P$ and $\xi \leq -\xi_* - 3$, then $g_2 = 1, f_0 = 1$ and

$$\mathcal{L}V(q,p,\xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 \leq -\frac{kN}{8D_{\max}^2} |\xi| + \frac{\beta_0 + \delta + \epsilon}{\beta} kN |\xi| + \frac{\beta_0}{\beta} K_1 + \frac{\beta_0 + \delta + \epsilon}{\beta} kN.$$

By choice of $\delta, \epsilon > 0$, we observe that $\frac{\beta_0 + \delta + \epsilon}{\beta} < \frac{1}{8D_{\max}^2}$, so by increasing $\xi_* > 0$ if necessary, we also arrive at the estimate

$$\mathcal{L}V(q,p,\xi) + \frac{\gamma}{\beta} |\nabla_p(V)|^2 \leq -\alpha$$

in the region $|p| \leq P$ and $\xi \leq -\xi_* - 3$. This finishes the proof. □

5. Smoothing and support properties

Here we establish conclusions (i) and (ii) of Proposition 2.1 separately.

Proof. (Proof of Proposition 2.1 (i).) We apply Corollary 7.2 of [35] and check that Hörmander’s bracket condition, as stated in relation (162) of [35], is satisfied on \mathcal{X} . See [20] for Hörmander’s original statement and proof. Letting \mathcal{L}^* denote the formal L^2 -adjoint of \mathcal{L} , this will then ensure hypoellipticity of the operators $\mathcal{L}, \mathcal{L}^*, \partial_t \pm \mathcal{L}, \partial_t \pm \mathcal{L}^*$ on the respective domains $\mathcal{X}, \mathcal{X}, (0, \infty) \times \mathcal{X}, (0, \infty) \times \mathcal{X}$. For $i \in \{1, 2, \dots, N\}$ and $\ell \in \{1, 2, \dots, k\}$, let $X_i^\ell = \partial_{p_i^\ell}$ and define

$$X_0 = \sum_{i=1}^N \frac{p_i}{m_i} \cdot \nabla_{q_i} - \sum_{i=1}^N \left(\xi + \frac{\gamma}{m_i} \right) p_i \cdot \nabla_{p_i} - \nabla U \cdot \nabla_p + a^{-1} (\|p\|_m^2 - kN/\beta) \partial_\xi.$$

Letting $[A, B] = AB - BA$ denote the commutator of operators A and B , we find that

$$[X_i^\ell, X_0] = m_i^{-1} \partial_{q_i^\ell} - (\xi + \gamma/m_i) \partial_{p_i^\ell} + \frac{2}{am_i} p_i^\ell \partial_\xi$$

and $[X_i^\ell, [X_i^\ell, X_0]] = \frac{2}{am_i} \partial_\xi$. Therefore, the list of vector fields

$$\begin{aligned} X_i^\ell, & \quad i = 1, 2, \dots, N, \ell = 1, 2, \dots, k \\ [X_i^\ell, X_0], & \quad i = 1, 2, \dots, N, \ell = 1, 2, \dots, k \\ [X_i^\ell, [X_i^\ell, X_0]], & \quad i = 1, 2, \dots, N, \ell = 1, 2, \dots, k \end{aligned}$$

has full rank at every point $x \in \mathcal{X}$. □

We next turn to the proof of Proposition 2.1 (ii) which relies on the support theorems [40, 41]. That is, to Equation (NHB) we associate a deterministic control problem on \mathcal{X}

$$\dot{Q}_i = \frac{P_i}{m_i}$$

$$\begin{aligned} \dot{P}_i &= -\Xi P_i - \frac{\gamma}{m_i} P_i - \nabla_{Q_i} U(Q) + \sqrt{2\gamma/\beta} \eta_i \\ \dot{\Xi} &= \sum_{i=1}^N \frac{|P_i|^2}{am_i} - \frac{kN}{a\beta} \end{aligned} \tag{5.1}$$

where $\eta = (\eta_i)$ is a piecewise continuous $(\mathbf{R}^k)^N$ -valued control and $\beta = 1/(k_B T)$. Intuitively for a fixed such η , the solution of (5.1) represents an approximate sample trajectory of the solution of (NHB). The support theorems [40, 41] make this intuition precise. In particular, for $x \in \mathcal{X}$ and $t > 0$ define $A(x, t)$ to be the set of points $y \in \mathcal{X}$ such that there exists a piecewise continuous $(\mathbf{R}^k)^N$ -valued control $\eta = (\eta_i)$ for which the solution of (5.1) exists on the time interval $[0, t]$ in \mathcal{X} and has $(Q(0), P(0), \Xi(0)) = x$ and $(Q(t), P(t), \Xi(t)) = y$. Then the support theorems [40, 41] imply that for every $x \in \mathcal{X}$ and every $t > 0$

$$\text{supp } \mathcal{P}_t(x, \cdot) = \text{closure}(A(x, t)). \tag{5.2}$$

Thus the problem of finding points in $\text{supp } \mathcal{P}_t(x, \cdot)$ can be cast in terms finding points reachable from the system (5.1) at exactly time $t > 0$ started at $x \in \mathcal{X}$ as the controls vary through the class of piecewise continuous functions.

REMARK 5.1. It is worth noting that solving the control problem above is slightly more involved than the one in the case of Langevin dynamics with uniformly elliptic noise in the momentum directions. One can see the difference between the two cases almost immediately, as the process solving (NHB) is not fully supported in \mathcal{X} instantaneously. Indeed, for all $t \geq 0$

$$\xi(t) \geq \xi(0) - ta^{-1}kN/\beta \quad \mathbf{P} - \text{a.s.}$$

In other words, the ξ process is only allowed to decrease so fast, hence restricting access to points at a given time $t > 0$ sufficiently far to the left of where it started. Although from this observation one is tempted to conjecture that for a given $x = (q, p, \xi) \in \mathcal{X}$ and $t > 0$

$$\text{supp } \mathcal{P}_t(x, \cdot) = \{(q', p', \xi') \in \mathcal{X} : \xi' \geq \xi - ta^{-1}k_B T k N\},$$

which is false. Consult the statement of Proposition 2.1 (ii) to see what precisely is claimed. Thus, determining the supports of the transitions, and hence solving the control problem (5.1), is more subtle.

While there are other methods, such as those from geometric control theory, that could prove useful in analyzing the problem above (see, for example, [11, 24] and the Agrachev-Sarachev approach as outlined in the infinite-dimensional setting in [39]), we choose to prove Proposition 2.1 (ii) by an essentially explicit construction. As seen below, we can recast the control problem as a calculus of variations problem.

Proof. (Proof of Proposition 2.1 (ii).) Let $x = (q, p, \xi) \in \mathcal{X}$ and $t > 0$. By the support theorems [40, 41], it suffices to prove that

$$\text{closure}(A(x, t)) = \mathcal{A}(x, t) \tag{5.3}$$

where $\mathcal{A}(x, t)$ is as in (2.13). To see the inclusion “ \subseteq ” in (5.3), let $\eta = (\eta_i)$ be an arbitrary piecewise continuous $(\mathbf{R}^k)^N$ -valued control such that the solution of (5.1)

with $(Q(0), P(0), \Xi(0)) = (q, p, \xi)$ exists in \mathcal{X} for all times on $[0, t]$. Letting $q' = Q(t)$ and $\xi' = \Xi(t)$, note by the Cauchy-Schwarz inequality

$$L_{q,q'}^2 \leq \left(\int_0^t \|P(u)\|_m du \right)^2 \leq t \int_0^t \|P(u)\|_m^2 du.$$

Consequently,

$$\begin{aligned} \xi' &= \xi + a^{-1} \int_0^t \|P(u)\|_m^2 du - ta^{-1}k_B T k N \\ &\geq \xi + \frac{L_{q,q'}^2}{ta} - ta^{-1}k_B T k N. \end{aligned}$$

This establishes the claimed inclusion. For the other inclusion “ \supseteq ” in (5.3), since \mathcal{O} is open let $\epsilon > 0$ be small enough so that $B_\epsilon(q) \subseteq \mathcal{O}$ and define $X_\epsilon = B_\epsilon(q) \times (\mathbf{R}^k)^N \times \mathbf{R}$. It suffices to show that

$$\text{closure}(A(x, t)) \cap X_\epsilon \supseteq \mathcal{A}(x, t) \cap X_\epsilon.$$

Note that this allows us to “convexify” the problem; that is, for any $q' \in B_\epsilon(q)$, $L_{q,q'} = \|q - q'\|_m$. Let $(q', p', \xi') \in X_\epsilon$ and $t > 0$. For a small parameter $\delta \in (0, t/2)$, consider the following piecewise linear curve $\phi_\delta : [0, t] \rightarrow (\mathbf{R}^k)^N$ given by

$$\phi_\delta(u) = \begin{cases} q + up & \text{if } 0 \leq u \leq \delta \\ \ell_u(q + \delta p, q' - \delta p') & \text{if } \delta \leq u \leq t - \delta \\ q' + (u - t)p' & \text{if } t - \delta \leq u \leq t. \end{cases}$$

where $u \mapsto \ell_u(q + \delta p, q' - \delta p')$ linearly interpolates between the points $q + \delta$ at time $u = \delta$ and $q' - \delta p'$ at time $u = t - \delta$. Observe that for any $\delta > 0$ sufficiently small, $\phi_\delta([0, t]) \subseteq B_\epsilon(q)$ and that for every $\delta > 0$, $\phi_\delta(0) = q, \dot{\phi}_\delta(0) = p, \phi_\delta(t) = q', \dot{\phi}_\delta(t) = p'$. Moreover, observe that as $\delta \rightarrow 0$

$$\int_0^t \|\dot{\phi}_\delta(u)\|_m^2 du \rightarrow \frac{\|q - q'\|_m^2}{t} = \frac{L_{q,q'}^2}{t}.$$

Thus by picking $\eta = (\eta_{i,\delta})$ to satisfy the second equation in (5.1) with this choice of $(Q, P) = (\phi_\delta, \dot{\phi}_\delta)$ proves that all points $(q', p', \xi') \in X_\epsilon$ with

$$\xi' = \xi + (at)^{-1}L_{q,q'}^2 - ta^{-1}k_B T k N$$

belong to $\text{closure}(A(x, t))$. To get the remaining points, first suppose that $q \neq q'$. For $s \in (0, t]$, define

$$\phi_\delta^s(u) = \begin{cases} q + up & \text{if } 0 \leq u \leq \delta \\ \ell_u(q + \delta p, q' - \delta p') & \text{if } \delta \leq u \leq s - \delta \\ q' - \delta p' & \text{if } s - \delta \leq u \leq t - \delta \\ q' + (u - t)p' & \text{if } t - \delta \leq u \leq t \end{cases}$$

where in the above, the $u \mapsto \ell_u(q_1, q_2)$ is the line segment connecting q_1 and q_2 at times $u = \delta$ and $u = s - \delta$. Note that for every $s \in (0, t]$, as $\delta \rightarrow 0$

$$\int_0^t \|\dot{\phi}_\delta^s(u)\|_m^2 du \rightarrow \frac{\|q - q'\|_m^2}{s} := f(s).$$

Since f is a continuous function of $s \in (0, t]$ with $f(t) = \|q - q'\|_m^2/t$ and $\lim_{s \downarrow 0} f(s) = \infty$, we can apply the Intermediate Value Theorem to see that all points $(q', p', \xi') \in X_\epsilon$ with $q' \neq q$ satisfying

$$\xi' > \xi + (at)^{-1}L_{q,q'}^2 - ta^{-1}k_B T k N$$

belong to $\text{closure}(A(x, t))$. Since $\text{closure}(A(x, t))$ is a closed set the result follows. \square

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Appendix. Here we use Theorem 2.2 and Proposition 2.1 to conclude Theorem 2.1. What follows is fairly standard but we provide the details for completeness. We first translate Theorem 2.2 and Proposition 2.1 to the following two corollaries which allow us to better connect with the setup in [14].

COROLLARY 6.1. *Let $\beta_0 > 0$ satisfy (2.12), fix $\epsilon \in (0, \beta_0)$ and let $W \in C^2(\mathcal{X})$ and $R, \alpha, K > 0$ satisfy (I) and (II) in Theorem 2.2. Then for all $t \geq 0$ and all $x \in \mathcal{X}$*

$$\mathcal{P}_t W(x) \leq e^{-\alpha t} W(x) + K/\alpha. \tag{6.4}$$

Proof. For $n \in \mathbf{N}$, define $\sigma_n = \inf\{t > 0 : W(x(t)) > n\}$ and let $\sigma_n(t) = t \wedge \sigma_n$. By construction of W , we see that $\mathbf{E}_x e^{\alpha \sigma_n(t)} (W(x_{\sigma_n(t)}) - K/\alpha) \leq W(x) - K/\alpha$, which in turn implies the estimate

$$\mathbf{E}_x e^{\alpha \sigma_n(t)} W(x_{\sigma_n(t)}) \leq W(x) + \mathbf{E}_x e^{\alpha \sigma_n(t)} K/\alpha. \tag{6.5}$$

Note that $\sigma_n \uparrow \infty$ \mathbf{P}_x -almost surely since $W(x) \rightarrow \infty$ as $H(x) \rightarrow \infty$ and $x(t)$ is non-explosive. Applying Fatou’s lemma and monotone convergence to (6.5) finishes the proof. \square

COROLLARY 6.2. *Let $\beta_0 > 0$ satisfy (2.12), fix $\epsilon \in (0, \beta_0)$ and let $W \in C^2(\mathcal{X})$ and $R, \alpha, K > 0$ satisfy (I) and (II) in Theorem 2.2. For $R > 0$, define*

$$\mathcal{C}_R = \{x \in \mathcal{X} : W(x) \leq R\}.$$

Then for each $R > 0$, \mathcal{C}_R is compact. Also, for each $R > 0$ large enough and each $t_0 > 0$, there exists a probability measure ν on Borel subsets of \mathcal{X} and a constant $c > 0$ such that for all $A \in \mathcal{B}(\mathcal{X})$

$$\inf_{x \in \mathcal{C}_R} \mathcal{P}_{t_0}(x, A) \geq c\nu(A). \tag{6.6}$$

Proof. The fact that \mathcal{C}_R is compact for $R > 0$ follows since $W(x) \rightarrow \infty$ as $H(x) \rightarrow \infty$, $W \in C^2(\mathcal{X}; (0, \infty))$ and since the potential U is normal. Let $R > 0$ be large enough so that $\mathcal{C}_R \neq \emptyset$ and fix $t_0 > 0$. First observe that for any $A \subseteq \mathcal{X}$ Borel and $x \in \mathcal{X}$ we may write

$$\mathcal{P}_{t_0}(x, A) = \int_A \int_{\mathcal{X}} r_{\frac{t_0}{2}}(x, y) r_{\frac{t_0}{2}}(y, z) dy dz \tag{6.7}$$

where we recall that $y \mapsto r_t(x, y)$ denotes the probability density of $\mathcal{P}_t(x, \cdot)$ with respect to Lebesgue measure on \mathcal{X} . From this expression, the goal is to now use support and regularity properties of the transitions to bound the quantity below by a positive constant times normalized Lebesgue measure on a bounded subset of \mathcal{X} . To this end, since \mathcal{C}_R is compact let

$$\xi_R = \max_{(q', p', \xi') \in \mathcal{C}_R} \xi' \quad \text{and} \quad L_R^2 = \max_{(q, p, \xi), (q', p', \xi') \in \mathcal{C}_R} L_{q, q'}^2$$

and note that by Proposition 2.1 (ii)

$$\mathcal{P}_{\frac{t_0}{2}}(x, B_\delta(y')) > 0$$

for all $x \in \mathcal{C}_R$, $\delta > 0$ and all $y' = (q', p', \xi') \in \mathcal{X}$ with

$$\xi' \geq \xi_R + (at_0/2)^{-1} L_R^2 - \frac{t_0}{2} a^{-1} k_B T k N.$$

Let $y' \in \mathcal{X}$ be any such point satisfying the above. Clearly, there exists $z' \in \mathcal{X}$ such that $r_{t_0/2}(y', z') > 0$. Employing continuity of the density on $(0, \infty) \times \mathcal{X} \times \mathcal{X}$ and picking $\delta > 0$ small enough we can ensure the following bound

$$r_{\frac{t_0}{2}}(y, z) \geq \epsilon > 0$$

for all $(y, z) \in B_\delta(y') \times B_\delta(z')$ where $\epsilon > 0$ is a constant. Hence by way of (6.7) we obtain for $x \in \mathcal{C}_R$

$$\mathcal{P}_{t_0}(x, A) \geq \epsilon \lambda(B_\delta(z')) \mathcal{P}_{\frac{t_0}{2}}(x, B_\delta(y')) \frac{\lambda(A \cap B_\delta(z'))}{\lambda(B_\delta(z'))}$$

where λ denotes Lebesgue measure. Since $x \mapsto \mathcal{P}_{\frac{t_0}{2}}(x, B_\delta(y'))$ is continuous and positive on \mathcal{C}_R , we infer the existence of a constant $c > 0$ such that

$$\inf_{x \in \mathcal{C}_R} \mathcal{P}_{t_0}(x, A) \geq c \frac{\lambda(A \cap B_\delta(z'))}{\lambda(B_\delta(z'))}$$

for all $A \subseteq \mathcal{X}$ Borel. This finishes the proof. □

We now use the previous two corollaries to conclude Theorem 2.1.

Proof. (Proof of Theorem 2.1.) We first show that the augmented Gibbs measure μ defined in relation (2.3) is an invariant probability measure for the Markov process $x(t)$ satisfying (NHB). Since U is a normal potential, μ is a probability measure by definition. Note also that it is a routine calculation to check that

$$\mathcal{L}^*(\exp(-\beta H)) = 0$$

where we recall that $\beta = 1/(k_B T)$ and \mathcal{L}^* is the formal L^2 -adjoint of the generator \mathcal{L} . This in turn implies that $\mu \mathcal{P}_t = \mu$ for all $t \geq 0$. To see that μ is unique, Proposition 2.1 (i) implies that $(\mathcal{P}_t)_{t \geq 0}$ is a strong Feller Markov semigroup. Moreover, we claim that $\text{supp } \nu = \mathcal{X}$ for any invariant probability measure ν for the Markov process $x(t)$. Uniqueness of μ will then follow by, for example, Theorem 3.16 of [13]. Supposing that ν is an invariant probability measure for $x(t)$, there exists $x^* \in \mathcal{X}$ for which $x^* \in$

$\text{supp } \nu$. By Proposition 2.1 (ii), for any $y \in \mathcal{X}$ we may pick $t > 0$ large enough so that $y \in \text{supp } \mathcal{P}_t(x^*, \cdot)$. Since for any $U, V \in \mathcal{B}(\mathcal{X})$

$$\nu(U) = \int_{\mathcal{X}} \nu(dx) \mathcal{P}_t(x, U) \geq \int_V \nu(dx) \mathcal{P}_t(x, U)$$

it follows that $y \in \text{supp } \nu$.

To obtain the remaining conclusions in the Theorem 2.1, we seek to apply Theorem 1.2 of [14] to the embedded Markov chain on \mathcal{X} given by $\mathcal{P}_n^{t_0} := \mathcal{P}_{nt_0}$ where $t_0 > 0$ is as in the statement of Corollary 6.2. Note that Corollary 6.1 and Corollary 6.2 together imply Assumption 1 and Assumption 2 of [14]. Applying Theorem 1.2 of [14], there exist constants $C > 0$ and $\delta \in (0, 1)$ such that

$$\rho_W(\nu_1 \mathcal{P}_n^{t_0}, \nu_2 \mathcal{P}_n^{t_0}) \leq C \delta^n \rho_W(\nu_1, \nu_2)$$

for all $\nu_i \in \mathcal{M}_W$ and all $n \in \mathbf{N} \cup \{0\}$. To reintroduce the continuous-time parameter $t > 0$ in the bound above, let $t = nt_0 + \epsilon$ for some $\epsilon \in (0, t_0)$ and $n \in \mathbf{N} \cup \{0\}$. Observe that for any $\varphi : \mathcal{X} \rightarrow \mathbf{R}$ measurable with $\|\varphi\|_W \leq 1$, Corollary 6.1 gives

$$\|\mathcal{P}_\epsilon \varphi\|_W \leq \|\varphi\|_W \sup_{x \in \mathcal{X}} \frac{1 + \mathcal{P}_\epsilon W(x)}{1 + W(x)} \leq C'$$

for some constant $C' > 0$ independent of $\epsilon > 0$. Applying Fubini-Tonelli and the Chapman-Kolmogorov equations, it then follows that

$$\rho_W(\nu_1 \mathcal{P}_t, \nu_2 \mathcal{P}_t) \leq C' \rho_W(\nu_1 \mathcal{P}_n^{t_0}, \nu_2 \mathcal{P}_n^{t_0}) \leq CC' \delta^n \rho_W(\nu_1, \nu_2).$$

Picking $\eta = -\frac{1}{t_0} \log \delta$ and $C'' = CC' / \delta^{1/t_0}$ produces the desired estimate

$$\rho_W(\nu_1 \mathcal{P}_t, \nu_2 \mathcal{P}_t) \leq C'' e^{-\eta t} \rho_W(\nu_1, \nu_2)$$

which is satisfied for all $t \geq 0$ and $\nu_i \in \mathcal{M}_W$. \square

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